Supplementary material for "Finding the stable structures of $N_{1-x}W_X$ with an *ab-initio* high-throughput approach"

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This is a listing of structures discussed in the main body of the paper, including space groups, lattice constants, Wyckoff positions of atoms, k-point mesh information, energy as computed by VASP, and enthalpy compared to the reference system of αN_2 and BCC W. Additionally, high symmetry points for the simple cubic body centered cubic Brillouin zones are shown.

I. COMPUTATIONAL DETAILS

All calculations done here used VASP[1–3] with PAW Potentials[4,5] and using the AFLOW automatic framework[6–8]. The general form of INCAR file used was

```
ISYM=2          # SYMMMETRY=ON
IBRION=2        # Relax with conjugate gradient (when appropriate)
PREC=Accurate   # avoid wrap around errors
ENMAX=560       # 1.4*ENMAX (400) of pseudopotentials
LREAL=.FALSE.   # reciprocal space projection technique
EDIFF=1E-6      # high accuracy required
ALGO=Fast       # ALGO = Fast
SYMPREC=1e-7    # Precise Symmetry
ISPIN=1         # SPIN=OFF
ISMEAR=-1       # Fermi broadening
SIGMA=0.0272    # About 0.002 Ry
```

The vdW-DF2[9] functional as implemented in VASP[10,11] was used to study the effect of van der Waals interactions. In this case we used the PBE[12] PAW potentials, and modified the INCAR file to include the lines:

```
LUSE_VDW = .TRUE. # Turn on the van der Waals functional
AGGAC = 0.0000    # Turn off the GGA part of the PBE correlation
GGA = ML          # Use rPW86 exchange
Zab_vdW = -1.8867 # With a parameter change
```

II. BRILLOUIN ZONES USED IN BAND STRUCTURE PLOTS

This section describes the high symmetry points and lines which label the phonon dispersion and band structure plots in the main paper.[13,14]

Table I describes and Figure 1 shows the Brillouin zone for a simple cubic lattice, used in the phonon dispersion of Fig. 5 and the electronic band structure plot of Fig. 6.

Table II describes and Figure 2 shows the Brillouin zone for a body centered cubic lattice, used in the electronic band structure plot of Fig. 14.

Table III describes and Figure 3 shows the Brillouin zone for the centered monoclinic N_3W_2 structure #35, which forms part of the convex hull in the N-W system. The notation is from Lax,[14] although we choose the unique monoclinic axis to be in the "b" direction, rather than "c." This was used in the plot of the electronic band structure in Fig. 11 in the main paper.

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14. ABSTRACT
This is a listing of structures discussed in the main body of the paper, including space groups lattice constants, Wycko positions of atoms, k-point mesh information, energy as computed by VASP, and enthalpy compared to the reference system of N2 and BCC W. Additionally, high symmetry points for the simple cubic body centered cubic Brillouin zones are shown.

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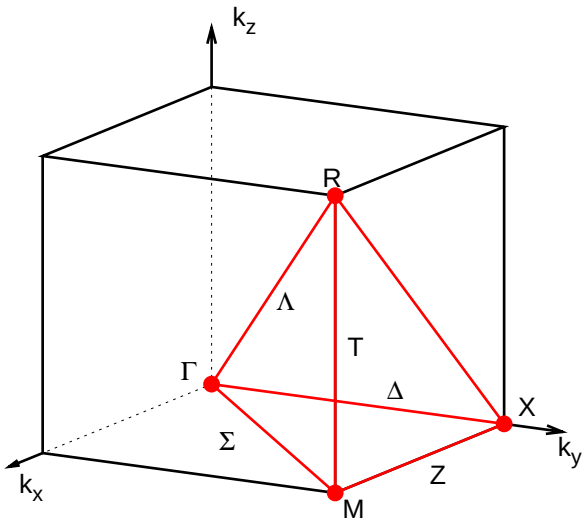

FIG. 1: 1/8 of the Brillouin zone of the simple cubic lattice, with high-symmetry points and directions labeled. The volume enclosed by the red lines is the irreducible part of the Brillouin zone. See Figs. 5 and 6 of the main paper.

TABLE I: Cartesian coordinates of the high symmetry points and lines in the Brillouin zone of a simple cubic lattice, following the notation presented in Lax.[14] The cubic lattice constant is a. The parameters x, y, and z range in value from 0 to 1.

Point	Coordinates	Line	Coordinates
Γ	$(0 , 0 , 0)$	Δ	$(0 , \frac{\pi}{a}y , 0)$
X	$(0 , \frac{\pi}{a} , 0)$	Σ	$(\frac{\pi}{a}x , \frac{\pi}{a}x , 0)$
M	$(\frac{\pi}{a} , \frac{\pi}{a} , 0)$	Λ	$(\frac{\pi}{a}x , \frac{\pi}{a}x , \frac{\pi}{a}x)$
R	$(\frac{\pi}{a} , \frac{\pi}{a} , \frac{\pi}{a})$	Z	$(\frac{\pi}{a}x , \frac{\pi}{a} , 0)$
		T	$(\frac{\pi}{a} , \frac{\pi}{a} , \frac{\pi}{a}z)$

Table IV describes and Figure 4 shows the Brillouin zone for the hexagonal MoS_2 structure (#89), which is near the convex hull at composition NW_2. The notation is from Lax.[14]

III. LOW ENERGY STRUCTURES IN THE W-N SYSTEM

The following sections give the equilibrium crystallographic information for the tungsten nitride structures plotted in Figures 1, 2 and 3 of the main paper. These structures were obtained by VASP, as described above. Results are given for each of the three functionals. Structures are arranged by composition, where x is the fraction of tungsten in the compound, *i.e.*, the composition is $N_{1-x}W_x$.

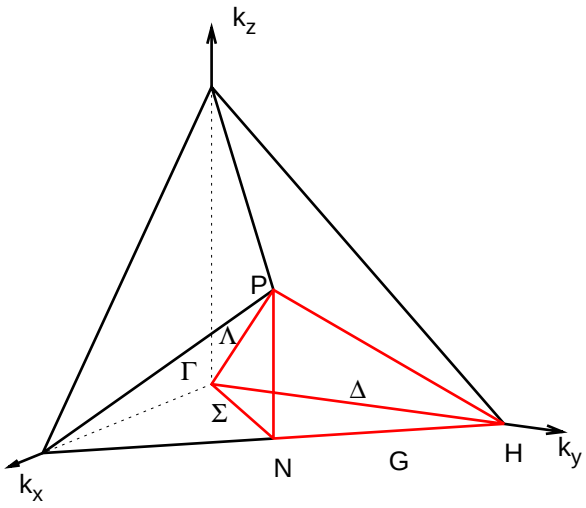

FIG. 2: 1/8 of the Brillouin zone of the body centered cubic lattice, with high-symmetry points and directions labeled. The volume enclosed by the red lines is the irreducible part of the Brillouin zone. See Fig. 14 of the main paper.

TABLE II: High symmetry points and lines in the Brillouin zone of a body centered cubic lattice, following the notation presented in Lax.[14] The cubic lattice constants a. The parameter x ranges in value from 0 to 1.

Point	Cartesian Coordinates
Γ	$(0 , 0 , 0)$
H	$(0 , \frac{2\pi}{a} , 0)$
N	$(\frac{\pi}{a} , \frac{\pi}{a} , 0)$
P	$(\frac{\pi}{a} , \frac{\pi}{a} , \frac{\pi}{a})$

Line	Cartesian Coordinates
Δ	$(0 , \frac{2\pi}{a}x , 0)$
Σ	$(\frac{\pi}{a}x , \frac{\pi}{a}x , 0)$
Λ	$(\frac{\pi}{a}x , \frac{\pi}{a}x , \frac{\pi}{a}x)$
G	$(\frac{\pi}{a}x , \frac{\pi}{a}(2-x) , 0)$

1. N_2 structures (x = 0)

Structure 1: Higher symmetry version of the two possible structures for αN_2.[15]

Space Group	$Pa\bar{3} - T_h^6$ (#205)			Pearson Symbol			$cP8$		
Functional	LDA			PBE			vdW-DF2		
a , b , c	5.22328Å	5.22328Å	5.22328Å	6.18740Å	6.18740Å	6.18740Å	5.51094Å	5.51094Å	5.51094Å
α , β , γ	90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:									
N (8c)	0.06094	0.06094	0.06094	0.05192	0.05192	0.05192	0.05814	0.05814	0.05814

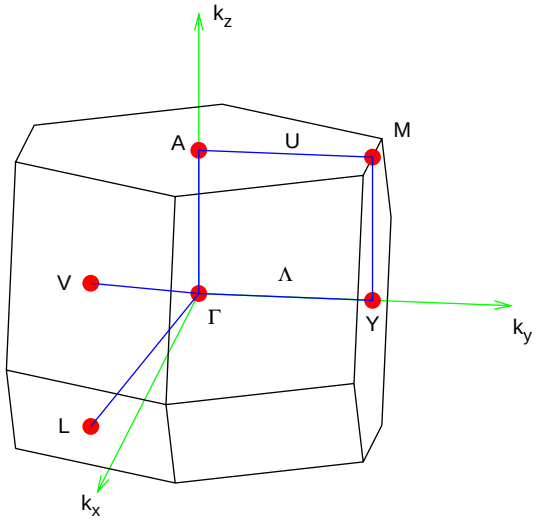

FIG. 3: Brillouin zone for the centered monoclinic structure #35, used to plot the electronic band structure in Figure 11 in the main paper. k_x, k_y, and k_z denote the Cartesian directions in reciprocal space. The labels are described in Table III. The blue lines represent the path taken for the band structure plot. Note that the reciprocal lattice primitive vectors are along the lines $\Gamma \to L$, $\Gamma \to Y$, and $\Gamma \to A$.

TABLE III: Real and reciprocal space primitive lattice vectors and high symmetry points for the centered monoclinic structure #35, following the notation of Lax.[14] The unique monoclinic axis is "b," and β is the angle between the other two primitive vectors in the full monoclinic lattice. A graphical depiction of the Brillouin zone is shown in Figure 3.

Real Space Primitive Vectors	
a_1 =	$(a , 0 , 0)$
a_2 =	$(a/2 , b/2, 0)$
a_3 =	$(c\cos\beta, 0 , c\sin\beta)$
Reciprocal Space Primitive Vectors	
b_1 =	$2\pi (1/a , -1/b , -\cot\beta/a)$
b_2 =	$2\pi (0 , 2/b , 0)$
b_3 =	$2\pi (0 , 0 , 1/(c\sin\beta))$
High symmetry points and lines (lattice coordinates)	
Γ	(0 , 0 , 0)
Y	(0 , 1/2 , 0)
A	(0 , 0 , 1/2)
L	(1/2 , 0 , 0)
V	(1/2 , 0 , 1/2)
M	(0 , 1/2 , 1/2)
Λ	(0 , y , 0)
U	(0 , y , 1/2)

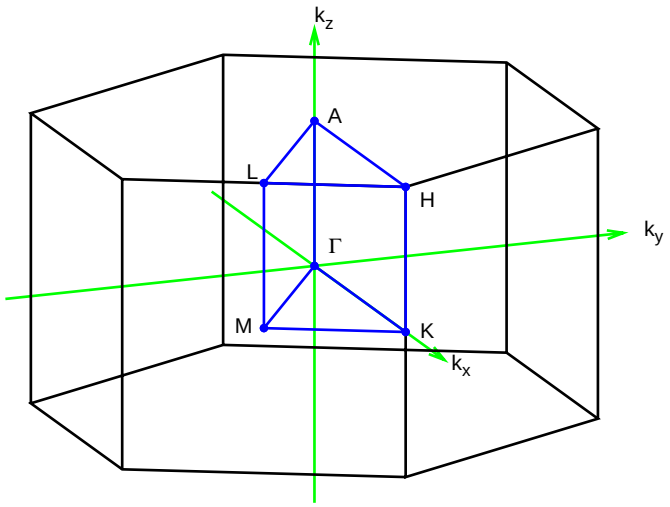

FIG. 4: Brillouin zone for the hexagonal lattice describing the MoS_2 structure (#89), with high-symmetry points and directions labeled. The volume enclosed by the red lines is the irreducible part of the Brillouin zone. See Figs. 17 of the main paper.

Structure 2: Lower symmetry version of the two possible structures for αN_2.[15]

Space Group	$P2_13 - T^4$ (#198)			Pearson Symbol			$cP8$		
Functional	LDA			PBE			vdW-DF2		
a , b , c	5.22293Å	5.22293Å	5.22293Å	6.18848Å	6.18848Å	6.18848Å	5.51064Å	5.51064Å	5.51064Å
α , β , γ	90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:									
N (4a)	0.18903	0.18903	0.18903	0.19903	0.19903	0.19903	0.19086	0.19086	0.19086
N (4a)	0.31093	0.31093	0.31093	0.30285	0.30285	0.30285	0.30714	0.30714	0.30714

Structure 3: Idealized version of the βN_2 structure.[15] In the real crystal the N_2 dimers are tilted away from the z axis and precess around it.

Space Group	$P6_3mmc - D^4_{6h}$(#194)			Pearson Symbol			$hP4$		
Functional	LDA			PBE			vdW-DF2		
a , b , c	3.54333Å	3.54333Å	6.75879Å	5.32369Å	5.32369Å	5.99005Å	3.37797Å	3.37797Å	8.17743Å
α , β , γ	90°	90°	120°	90°	90°	120°	90°	90°	120°
Wyckoff Positions:									
N (4f)	1/3	2/3	0.16836	1/3	2/3	0.15710	1/3	2/3	0.18210

TABLE IV: Real and reciprocal space primitive lattice vectors and high symmetry points for the hexagonal MoS_2 structure (#89) following the notation of Lax.[14] A graphical depiction of the Brillouin zone is shown in Figure 4.

Real Space Primitive Vectors	
a_1 =	($a/2$, $-\sqrt{3}a/2$, 0)
a_2 =	($a/2$, $\sqrt{3}a/2$, 0)
a_3 =	(0 , 0 , c)
Reciprocal Space Primitive Vectors	
b_1 =	2π ($1/a$, $-1/(\sqrt{3}a)$, 0)
b_2 =	2π ($1/a$, $1/(\sqrt{3}a)$, 0)
b_3 =	2π (0 , 0 , $1/c$)
High symmetry points and lines (lattice coordinates)	
Γ	(0 , 0 , 0)
M	(1/2 , 0 , 0)
K	(1/3 , 1/3 , 0)
A	(0 , 0 , 1/2)
L	(1/2 , 0 , 1/2)
H	(1/3 , 1/3 , 1/2)
Σ	(x , 0 , 0)
Λ	(x , x , 0)
Δ	(0 , 0 , z)
T	(1/2 - y/2, y , 0)
S	(1/2 - y/2, y , 1/2)

Structure 4: The γN_2 structure.[15]

Space Group	$P4_2/mnm - D^{14}_{4h}$ (#136)			Pearson Symbol			$tP4$		
Functional	LDA			PBE			vdW-DF2		
a , b , c	3.70846Å	3.70846Å	4.97143Å	4.42366Å	4.42366Å	6.00037Å	5.00815Å	5.00815Å	3.40798Å
α , β , γ	90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:									
N (4f)	0.10517	0.10517	0	0.08895	0.08895	0	0.07835	0.07835	0

Structure 5: The εN_2 structure.[16]

Space Group	$R\bar{3}c - D^6_{3d}$ (#167)			Pearson Symbol			$hR48$		
Functional	LDA			PBE			vdW-DF2		
a , b , c	8.80174Å	8.80174Å	12.24907Å	10.79199Å	10.79199Å	14.22027Å	7.77983Å	7.77983Å	16.59770Å
α , β , γ	90°	90°	120°	90°	90°	120°	90°	90°	120°
Wyckoff Positions:									
N (12c)	0	0	0.04502	0	0	0.03913	0	0	0.03343
N (36f)	0.26506	0.05772	0.27717	0.26603	0.04851	0.27269	0.24829	0.23172	0.28275

2. N_4W structures (x = 0.200)

Structure 6: N_4W in the ReP_4 structure,[17] as suggested by Aydin *et al.*[18] These are the lowest energy structures currently found for any N_4W structures with space group *Pbca* and all atoms at (8c) Wyckoff positions.

Space Group		$Pbca - D_{2h}^{15}$ (#61)			Pearson Symbol			$oP40$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		6.57765Å	7.31355Å	10.04929Å	6.32908Å	9.47153Å	16.40328Å	6.41544Å	9.53957Å	14.15573Å
α , β , γ		90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:										
N	(8c)	0.00000	0.27146	0.19455	0.00684	0.06754	0.31612	0.00948	0.06813	0.81845
N	(8c)	0.00000	0.22834	0.30561	0.00009	-0.00031	-0.07843	0.00003	-0.00057	0.40825
N	(8c)	0.21155	0.08492	-0.00002	0.00720	0.45044	0.18487	0.00965	0.04754	0.17993
N	(8c)	0.28845	0.08491	0.50002	0.24570	0.25182	0.50006	0.25847	0.25398	0.00006
W	(8c)	0.00000	0.29197	0.00003	0.00247	0.14512	-0.00014	0.00469	0.35392	-0.00031

Structure 7: N_4W in the ReP_4 structure,[17] as suggested by Aydin *et al.*[18] In each of these calculations the starting point was the LDA equilibrium structure found in Ref. 18, and the reported structures are the output of VASP without any additional processing.

Space Group		$Pbca - D_{2h}^{15}$ (#61)			Pearson Symbol			$oP40$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		5.31299Å	7.32999Å	9.09288Å	5.79944Å	7.48219Å	9.04380Å	5.04489Å	8.51604Å	11.67151Å
α , β , γ		90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:										
N	(8c)	0.17832	0.70716	0.27445	0.18619	0.29452	0.72720	0.17025	0.29833	0.31873
N	(8c)	0.28959	0.02740	0.27957	0.21599	0.02672	0.21965	0.22506	0.06813	0.82587
N	(8c)	0.19628	0.44795	0.13809	0.18529	0.55601	0.86490	0.23836	0.58417	0.04826
N	(8c)	0.17762	0.77908	0.13915	0.19658	0.27512	0.36690	0.07611	0.30939	0.54074
W	(8c)	0.33803	0.38254	0.44519	0.34946	0.61353	0.54802	0.33291	0.60732	0.43686

Structure 8: This is a derivative of the metastable FeB_4 structure proposed by Van der Geest and Kolmogorov.[19] A transcription error led to a lower energy structure for N_4W than the proposed FeB_4 structure. That structure was unstable with respect to a zone boundary phonon. We minimized the total energy of the unstable mode, leading to this structure.

Space Group		$Fmmm - D_{2h}^{23}$ (#69)			Pearson Symbol			$oF40$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		10.15460Å	5.90244Å	8.33310Å	10.27687Å	6.06425Å	8.38901Å	10.41306Å	6.23340Å	8.45489Å
α , β , γ		90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:										
N	(8i)	0	0	0.16221	0	0	0.16092	0	0	0.16011
N	(8i)	0	0	0.31099	0	0	0.31019	0	0	0.30870
N	(16o)	0.19332	0.25932	0	0.19364	0.26016	0	0.19440	0.26085	0
W	(8h)	0	0.27394	0	0	0.27660	0	0	0.27799	0

3. N_3W structures (x = 0.250)

Structure 9: The Molybdite (MoO_3) structure.[20]

Space Group		$Pnma - D_{2h}^{16}$ (#62)			Pearson Symbol			$oP16$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		18.23290Å	4.00463Å	2.86311Å	21.19384Å	4.05147Å	2.92603Å	19.58109Å	4.11494Å	2.98244Å
α , β , γ		90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:										
N	(4c)	0.46239	1/4	0.26162	0.20877	1/4	0.29389	0.45461	1/4	0.25942
N	(4c)	0.20253	1/4	0.79434	0.43523	1/4	0.78159	0.20504	1/4	0.78507
N	(4c)	0.40064	1/4	0.26712	0.38185	1/4	0.78348	0.39695	1/4	0.26382
W	(4c)	0.28911	1/4	0.29316	0.28388	1/4	0.29339	0.28834	1/4	0.28412

Structure 10: The P_3Tc structure,[21] also considered by Song and Wang.[22]

Space Group		$Pnma - D_{2h}^{16}$ (#62)			Pearson Symbol			$oP16$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		12.57592Å	2.88205Å	5.10810Å	12.65081Å	2.93872Å	5.28463Å	13.01170Å	3.03920Å	5.14367Å
α , β , γ		90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:										
N	(4c)	0.06859	1/4	0.66002	0.56590	1/4	0.66312	0.06580	1/4	0.67597
N	(4c)	0.47678	1/4	0.78395	0.47325	1/4	0.70824	0.47575	1/4	0.77887
N	(4c)	0.23098	1/4	0.23775	0.23395	1/4	0.23991	0.23002	1/4	0.24851
W	(4c)	0.33344	1/4	0.95416	0.33111	1/4	0.52096	0.33258	1/4	0.96251

4. N_2W structures (x = 0.33333)

Structure 11: The lower symmetry N_2W structure proposed by Wang *et al.*[23] This can be constructed from the WC structure (#61) by doubling the unit cell in the z direction and removing one of the tungsten atoms.

Space Group		$P\bar{6}m2 - D_{3h}^{1}$ (#187)			Pearson Symbol			$hP3$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		2.88726Å	2.88726Å	3.87688Å	2.93342Å	2.93342Å	3.91819Å	2.99962Å	2.99962Å	3.97445Å
α , β , γ		90°	90°	120°	90°	90°	120°	90°	90°	120°
Wyckoff Positions:										
N	(2g)	0	0	0.18044	0	0	0.18136	0	0	0.18238
W	(1d)	1/3	2/3	1/2	1/3	2/3	1/2	1/3	2/3	1/2

Structure 12: The higher symmetry N_2W structure proposed by Wang *et al.*[23]

Space Group		$P6_3/mmc - D_{6h}^{h}$ (#194)			Pearson Symbol			$hP4$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		2.89316Å	2.89316Å	7.71367Å	2.93922Å	2.93922Å	7.79617Å	3.00734Å	3.00734Å	7.89061Å
α , β , γ		90°	90°	120°	90°	90°	120°	90°	90°	120°
Wyckoff Positions:										
N	(4e)	0	0	0.08978	0	0	0.09016	0	0	0.09066
W	(2d)	1/3	2/3	3/4	1/3	2/3	3/4	1/3	2/3	3/4

Structure 13: N_2W in the high-temperature (β) tridymite SiO_2 structure.[24]

Space Group	$P6_3/mmc - D^4_{6h}$ (#194)			Pearson Symbol			$hP12$		
Functional	LDA			PBE			vdW-DF2		
a , b , c	6.01620Å	6.01620Å	9.77913Å	6.07821Å	6.07821Å	9.89100Å	6.14395Å	6.14395Å	9.98375Å
α , β , γ	90°	90°	120°	90°	90°	120°	90°	90°	120°
Wyckoff Positions:									
N (2c)	1/3	2/3	1/4	1/3	2/3	1/4	1/3	2/3	1/4
N (6g)	1/2	0	0	1/2	0	0	1/2	0	0
W (2d)	1/3	2/3	0.06202	1/3	2/3	0.06213	1/3	2/3	0.06200

Structure 14: N_2W in an idealized high-temperature (β) cristobalite SiO_2 structure.[25]

Space Group	$Fd\bar{3}m - O^7_h$ (#227)			Pearson Symbol			$cF24$		
Functional	LDA			PBE			vdW-DF2		
a , b , c	8.49553Å	8.49553Å	8.49553Å	8.58600Å	8.58600Å	8.58600Å	8.67534Å	8.67534Å	8.67534Å
α , β , γ	90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:									
N (16c)	0	1/4	1/4	0	1/4	1/4	0	1/4	1/4
W (4a)	1/8	1/8	1/8	1/8	1/8	1/8	1/8	1/8	1/8

Structure 15: N_2W constructed by removing 4 N and 10 W atoms from a cI64 supercell of the NaCl structure. Note that this structure can be considered as either a β phase or an SiO_2-like phase.

Space Group	$Im\bar{3}m - O^9_h$ (#229)			Pearson Symbol			$cI36$		
Functional	LDA			PBE			vdW-DF2		
a , b , c	10.27372Å	10.27372Å	10.27372Å	10.38300Å	10.38300Å	10.38300Å	10.49032Å	10.49032Å	10.49032Å
α , β , γ	90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:									
N (24h)	0	0.14537	0.14537	0	0.14546	0.14546	0	0.14553	0.14553
W (12d)	1/2	1/4	0	1/2	1/4	0	1/2	1/4	0

Structure 16: N_2W in the high-temperature β-quartz (SiO_2) structure.[26]

Space Group	$P6_222 - D^4_6$ (#180)			Pearson Symbol			$hP9$		
Functional	LDA			PBE			vdW-DF2		
a , b , c	5.80091Å	5.80091Å	6.39312Å	5.86952Å	5.86952Å	6.46501Å	5.91904Å	5.91904Å	6.53442Å
α , β , γ	90°	90°	120°	90°	90°	120°	90°	90°	120°
Wyckoff Positions:									
N (6j)	0.21156	0.42312	1/2	0.21994	0.42388	1/2	0.21103	0.42206	1/2
W (3c)	1/2	0	0	1/2	0	0	1/2	0	0

Structure 17: N_2W starting from the β-NbO_2 structure (Space group $I4_1$, $tI48$).[27] This system relaxed to the smaller unit cell shown below. Both systems are distorted rutile structures.[28] The current system reduces to rutile when the z coordinate of the (4a) and (4c) sites both approach zero. The origin was chosen so that $z = 0$ for the tungsten atom.

Space Group	$P4_2nm - C_{4v}^4$ (#102)			Pearson Symbol			$tP6$		
Functional	LDA			PBE			vdW-DF2		
a , b , c	4.78575Å	4.78575Å	3.01573Å	4.85220Å	4.85220Å	3.06777Å	4.90940Å	4.90940Å	3.14841Å
α , β , γ	90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:									
N (4c)	0.29604	0.29604	0.10545	0.20347	0.20347	0.11185	0.20208	0.20208	0.11748
W (2a)	0	0	0	0	0	0	0	0	0

Structure 18: N_2W in the Brookite structure of TiO_2,[28] with N on the O sites. This was studied by Kroll, Schröter and Peters.[29]

Space Group	$Pbca - D_{2h}^{15}$ (#61)			Pearson Symbol			$oP24$		
Functional	LDA			PBE			vdW-DF2		
a , b , c	9.61612Å	4.88812Å	5.09072Å	9.77240Å	4.95123Å	5.16705Å	9.97738Å	5.03075Å	5.28028Å
α , β , γ	90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:									
N (8c)	0.96672	0.66613	0.67774	0.96657	0.66855	0.67720	0.96633	0.17410	0.67556
N (8c)	0.71228	0.74415	0.58230	0.71325	0.74383	0.58067	0.71463	0.24276	0.57564
W (8c)	0.64390	0.43772	0.82796	0.64349	0.43740	0.82628	0.64258	0.93919	0.82146

Structure 19: N_2W in the Mo_2N structure.[30] Note that although the composition of the experimental structure is actually $Mo_2N_{0.76}$ we treat both sites as fully occupied. Also note that in the special case $c = 2a$ and $z = 1/4$ majority atoms occupy all of the Na sites of the NaCl structure, while the minority atoms occupy half of the Cl sites, the remainder being vacant. This is therefore a highly relaxed variation of the β-NW structure.

Space Group	$I4_1/amd - D_{4h}^{19}$ (#141)			Pearson Symbol			$tI12$		
Functional	LDA			PBE			vdW-DF2		
a , b , c	3.74217Å	3.74217Å	10.51044Å	3.79214Å	3.79214Å	10.63734Å	3.84575Å	3.84575Å	10.80904Å
α , β , γ	90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:									
N (8e)	0	3/4	0.92786	0	3/4	0.92784	0	3/4	0.92773
W (4a)	0	3/4	1/8	0	3/4	1/8	0	3/4	1/8

Structure 20: The $CoSb_2$ structure.[31] This was also studied by Song and Wang,[22] although they refer to the structure as IrP_2, and is related to the Baddeleyite structure studied by Kroll, Schröter and Peters[29].

Space Group	$P2_1/c - C_{2h}^5$ (#14)			Pearson Symbol			$mP12$		
Functional	LDA			PBE			vdW-DF2		
a , b , c	4.85002Å	4.89988Å	5.12147Å	5.76275Å	4.82454Å	5.82063Å	5.84252Å	4.93943Å	5.93500Å
α , β , γ	90°	99.3565°	90°	90°	117.69846°	90°	90°	117.06754°	90°
Wyckoff Positions:									
N (4e)	0.43463	0.32878	0.16170	0.41323	0.80519	0.10053	0.40642	0.81372	0.09795
N (4e)	0.07383	0.73977	0.51917	0.09245	0.20634	0.40763	0.08940	0.20214	0.39837
W (4e)	0.21230	0.06261	0.28069	0.23917	0.49150	0.28846	0.23709	0.49323	0.29358

Structure 21: N_2W in the PbO_2 structure,[32] with N on the O sites. This is mostly notable because N_2W and PbO_2 have the same number of valence electrons per formula unit.

Space Group	$Pbcn - D_{2h}^{14}$ (#60)			Pearson Symbol			$oP12$		
Functional	LDA			PBE			vdW-DF2		
a , b , c	4.61441Å	5.73881Å	4.95802Å	4.66423Å	5.87309Å	5.02052Å	4.71366Å	6.04846Å	5.11078Å
α , β , γ	90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:									
N (8d)	0.22980	0.38025	0.58267	0.23167	0.37854	0.58254	0.23535	0.37674	0.58285
W (4c)	0	0.31384	1/4	0	0.31140	1/4	0	0.30751	1/4

Structure 22: N_2W structure derived from the r-W_2N_3 structure of Wang, Yu, Lin, *et al.*[33] (hereafter WYL+) by removing selected tungsten atoms, as described in the text. We use the freedom allowed by this space group to arbitrarily set the position of the W (2a) atom at the origin.

Space Group	$Cm - C_s^3$ (#8)			Pearson Symbol			$mC18$		
Functional	LDA			PBE			vdW-DF2		
a , b , c	5.13933Å	8.66309Å	4.53491Å	5.35271Å	8.70881Å	4.70314Å	5.48894Å	8.88675Å	4.79412Å
α , β , γ	90°	88.68574°	90°	90°	85.21917°	90°	90°	84.68995°	90°
Wyckoff Positions:									
N (2a)	0.39885	0	0.28915	0.45359	0	0.32740	0.45343	0	0.33761
N (2a)	0.72187	0	0.76307	0.73651	0	0.79298	0.74015	0	0.80716
N (4b)	0.21890	0.84377	0.77108	0.22590	0.84475	0.77894	0.21793	0.84287	0.77656
N (4b)	0.39471	0.33385	0.28086	0.41407	0.33275	0.29726	0.40545	0.33136	0.30077
W (2a)	0	0	0	0	0	0	0	0	0
W (4b)	0.01012	0.32851	0.51580	0.02443	0.32068	0.53208	0.01497	0.31785	0.53084

Structure 23: N_2W in the $PbCl_2$ (Cotunnite) structure.[34] Kroll, Schröter and Peters[29] predict this to be a high-pressure phase of N_2W.

Space Group	$Pnma - D_{2h}^{16}$ (#62)			Pearson Symbol			$oP12$		
Functional	LDA			PBE			vdW-DF2		
a , b , c	5.37104Å	3.09646Å	6.27663Å	5.43867Å	3.15265Å	6.36094Å	5.52840Å	3.24172Å	6.48041Å
α , β , γ	90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:									
N (4c)	0.03002	1/4	0.34564	0.02840	1/4	0.34659	0.02522	1/4	0.34743
N (4c)	0.13884	1/4	-0.07144	0.13885	1/4	-0.07226	0.13838	1/4	-0.07373
W (4c)	0.26124	1/4	0.62346	0.26082	1/4	0.62185	0.25932	1/4	0.61880

Structure 24: N_2W in the CTi_2 structure.[35] This is the reverse of the structure #95.

Space Group	$Fd\bar{3}m - O_h^7$ (#227)			Pearson Symbol			$hR33$		
Functional	LDA			PBE			vdW-DF2		
a , b , c	8.43254Å	8.43254Å	8.43254Å	8.56458Å	8.56458Å	8.56458Å	8.72077Å	8.72077Å	8.72077Å
α , β , γ	90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:									
N (32e)	0.23809	0.23809	0.23809	0.23740	0.23740	0.23740	0.23658	0.23658	0.23658
W (16c)	0	0	0	0	0	0	0	0	0

Structure 25: N_2W in the αSm structure.[36] This is the the structure Khitrova and Pinsker[37] call δ_R^V, and is the reverse of structure 91.

Space Group	$R\bar{3}m - D_{3d}^5$ (#166)			Pearson Symbol			$hR9$		
Functional	LDA			PBE			vdW-DF2		
a , b , c	2.98981Å	2.98981Å	14.05631Å	3.02518Å	3.02518Å	16.63670Å	3.09742Å	3.09742Å	14.65992Å
α , β , γ	90°	90°	120°	90°	90°	120°	90°	90°	120°
Wyckoff Positions:									
N (6c)	0	0	0.25981	0	0	0.27042	0	0	0.26261
W (3a)	0	0	0	0	0	0	0	0	0

Structure 26: N_2W in a structure proposed by Du, Wang, and Lo.[38] While the original reference found a six atom unit cell, we found that the structure they gave reduces to the three atom primitive cell described below.

Space Group	$P4/mmm - D_{4h}^1$ (#123)			Pearson Symbol			$tP3$		
Functional	LDA			PBE			vdW-DF2		
a , b , c	2.67640Å	2.67640Å	3.64237Å	2.71816Å	2.71816Å	3.69124Å	2.77942Å	2.77942Å	3.76517Å
α , β , γ	90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:									
N (2h)	1/2	1/2	0.30958	1/2	1/2	0.30936	1/2	1/2	0.31038
W (1a)	0	0	0	0	0	0	0	0	0

Structure 27: N_2W constructed by removing 16 W atoms from a cP64 supercell of the NaCl structure.

Space Group	$Pm\bar{3}m - O_h^1$ (#221)			Pearson Symbol			$cI36$		
Functional	LDA			PBE			vdW-DF2		
a , b , c	8.37235Å	8.37235Å	8.37235Å	8.50430Å	8.50430Å	8.50430Å	8.64939Å	8.64939Å	8.64939Å
α , β , γ	90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:									
N (6e)	0	0	0.24188	0	0	0.24115	0	0	0.23985
N (6f)	0.22121	1/2	1/2	0.21951	1/2	1/2	0.22014	1/2	1/2
N (8g)	0.22503	0.22503	0.22503	0.22368	0.22368	0.22368	0.22274	0.22274	0.22274
N (12h)	0.24919	0	1/2	0.25006	0	1/2	0.25019	0	1/2
W (1a)	0	0	0	0	0	0	0	0	0
W (3c)	0	1/2	1/2	0	1/2	1/2	0	1/2	1/2
W (12i)	0	0.27161	0.27161	0	0.27227	0.27227	0	0.27298	0.27298

Structure 28: N_2W constructed by removing 16 W atoms from a cP64 supercell of the NaCl structure. Note that this subset is orthogonal to the set chosen in Structure 27.

Space Group		$Pm\bar{3}m - O_h^1$ (#221)			Pearson Symbol			$cI36$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		8.32293Å	8.32293Å	8.32293Å	8.47983Å	8.47983Å	8.47983Å	8.64745Å	8.64745Å	8.64745Å
α , β , γ		90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:										
N	(6e)	0	0	0.23176	0	0	0.22945	0	0	0.22961
N	(6f)	0.24399	1/2	1/2	0.23970	1/2	1/2	0.23409	1/2	1/2
N	(8g)	0.27168	0.27168	0.27168	0.27168	0.27618	0.27618	0.27862	0.27862	0.27862
N	(12h)	0.24802	0	1/2	0.24869	0	1/2	0.24928	0	1/2
W	(1a)	0	0	0	0	0	0	0	0	0
W	(3c)	0	1/2	1/2	0	1/2	1/2	0	1/2	1/2
W	(12j)	1/2	0.22881	0.22881	1/2	0.22696	0.22696	1/2	0.22425	0.22425

5. $N_{16}W_9$ structures (x = 0.360)

Structure 29: $N_{16}W_9$ in the δ_H^{IV} structure of Khitrova and Pinsker,[37] constructing a $2 \times 2 \times 1$ supercell of the parent structure (#64) and then removing all but one of the atoms from the second set of W (2b) images. The cell is shifted to put the first nitrogen atom at the origin.

Space Group		$P3m1 - C_{3v}^1$ (#156)			Pearson Symbol			$hP25$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		5.92297Å	5.92297Å	9.56224Å	6.00383Å	6.00383Å	9.80913Å	6.15469Å	6.15469Å	9.85228Å
α , β , γ		90°	90°	120°	90°	90°	120°	90°	90°	120°
Wyckoff Positions:										
N	(1a)	0	0	0	0	0	0	0	0	0
N	(1b)	1/3	2/3	0.23958	1/3	2/3	0.23766	1/3	2/3	0.23266
N	(1b)	1/3	2/3	0.71140	1/3	2/3	0.70805	1/3	2/3	0.70366
N	(1c)	2/3	1/3	0.50027	2/3	1/3	0.50316	2/3	1/3	0.50377
N	(3d)	0.50255	0.00509	0.01443	0.50249	0.00497	0.01846	0.50215	0.00429	0.01513
N	(3d)	0.33217	0.16609	0.25173	0.33205	0.16603	0.25266	0.33168	0.16584	0.24812
N	(3d)	0.16435	0.32870	0.49064	0.16558	0.33115	0.49060	0.16758	0.33515	0.48703
N	(3d)	0.33344	0.16672	0.72475	0.32944	0.16472	0.72286	0.32488	0.16244	0.71952
W	(1a)	0	0	0.36105	0	0	0.35888	0	0	0.35337
W	(1a)	0	0	0.79739	0	0	0.79696	0	0	0.79342
W	(1c)	2/3	1/3	0.14820	2/3	1/3	0.15220	2/3	1/3	0.15671
W	(3d)	0.17464	0.34929	0.11930	0.17454	0.34908	0.11994	0.17637	0.35275	0.11232
W	(3d)	0.49577	0.99154	0.59760	0.49519	0.99039	0.59605	0.49451	0.98902	0.59183

6. N_8W_5 structures (x = 0.38462)

Structure 30: N_8W_5 in the δ_H^{III} structure of Khitrova and Pinsker,[37] constructing a $2 \times 2 \times 1$ supercell of the parent structure (#58 and then removing six tungsten atoms from the tungsten (2a) sites, including all four atoms in the $z = 1/2$ plane.

Space Group		$P2/m - C_{2h}^1$ (#10)			Pearson Symbol			$mP13$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		4.98468Å	2.83670Å	9.44454Å	5.06191Å	2.87834Å	9.56504Å	5.16975Å	2.94390Å	9.71586Å
α , β , γ		90°	101.65647°	90°	90°	101.79558°	90°	90°	101.90217°	90°
Wyckoff Positions:										
N	(2m)	0.35984	0	0.15177	0.35840	0	0.15236	0.35713	0	0.15306
N	(2m)	0.47276	0	0.42551	0.47209	0	0.42536	0.47147	0	0.42519
N	(2n)	0.02821	1/2	0.57430	0.02852	1/2	0.57448	0.02848	1/2	0.57460
N	(2n)	0.87270	1/2	0.14872	0.87183	1/2	0.14919	0.87267	1/2	0.15053
W	(2a)	0	0	0	0	0	0	0	0	0
W	(2m)	0.09101	0	0.29409	0.09039	0	0.29442	0.09040	0	0.29558
W	(2n)	0.58361	1/2	0.28467	0.58242	1/2	0.28491	0.58167	1/2	0.28466

Structure 31: N_8W_5 constructed by removing W atoms from the base r-W_2N_3 structure (#63).

Space Group		$R3m - C_{3v}^5$ (#160)			Pearson Symbol			$hR39$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		5.78224Å	5.78224Å	14.83815Å	5.85783Å	5.85783Å	15.10903Å	5.97504Å	5.97504Å	15.33870Å
α , β , γ		90°	90°	120°	90°	90°	120°	90°	90°	120°
Wyckoff Positions:										
N	(3a)	0	0	0.41651	0	0	0.41705	0	0	0.41602
N	(3a)	0	0	0.57783	0	0	0.57735	0	0	0.57669
N	(9b)	0.17772	0.35545	0.75519	0.17813	0.35625	0.75559	0.17918	0.35836	0.75627
N	(9b)	0.34356	0.17178	0.25399	0.34492	0.17246	0.25379	0.34805	0.17402	0.25397
W	(3a)	0	0	-0.00645	0	0	-0.00676	0	0	-0.00661
W	(3a)	0	0	0.18136	0	0	0.18126	0	0	0.18321
W	(9b)	0.16162	0.32324	0.49707	0.16108	0.32215	0.49699	0.16005	0.32011	0.49599

Structure 32: N_8W_5 in the δ_H^{III} structure of Khitrova and Pinsker,[37] constructing a $2 \times 2 \times 1$ supercell of the parent structure (#58 and then removing three tungsten atoms from each of the $z = 0$ and the $z = 1/2$ tungsten (2a) sites, leaving two atoms which are not stacked on top of one another.

Space Group		$Cmca - D_{2h}^{18}$ (#64)			Pearson Symbol			$oC52$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		5.76208Å	9.96021Å	10.17893Å	5.83772Å	10.10123Å	10.35710Å	5.95593Å	10.30294Å	10.47476Å
α , β , γ		90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:										
N	(8f)	0	0.15690	0.12857	0	0.15663	0.12816	0	0.15624	0.12823
N	(8f)	0	0.17150	0.36577	0	0.17174	0.36395	0	0.17185	0.36453
N	(16g)	0.26837	0.07914	0.62751	0.26851	0.07826	0.62788	0.26898	0.07761	0.62771
W	(4a)	0	0	0	0	0	0	0	0	0
W	(8e)	1/4	0.25002	1/4	1/4	0.25027	1/4	1/4	0.25037	1/4
W	(8f)	0	0.50021	0.23228	0	0.50279	0.23295	0	0.50037	0.23074

Structure 33: N_8W_5 in the δ_H^{IV} structure of Khitrova and Pinsker,[37] constructing a $2 \times 2 \times 1$ supercell of the parent structure (#64) and then removing six tungsten atoms from the images of the second W (2b) site, leaving one atom in each plane. We shift the origin so that the first nitrogen atom is at $z = 0$.

Space Group		$Cmc2_1 - C_{2v}^{12}$ (#36)			Pearson Symbol			$oC52$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		5.88119Å	10.18620Å	9.96161Å	5.95287Å	10.31069Å	10.19299Å	6.06601Å	10.50639Å	10.41632Å
α , β , γ		90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:										
N	(4a)	0	0.01292	0	0	0.01202	0	0	0.01051	0
N	(4a)	0	0.50008	0.04042	0	0.50015	0.04421	0	0.50024	0.04834
N	(4a)	0	0.67514	0.24156	0	0.67507	0.24152	0	0.67569	0.24124
N	(4a)	0	0.16663	0.26801	0	0.16671	0.26850	0	0.16678	0.26919
N	(8b)	0.23769	0.91277	0.24145	0.23771	0.91283	0.24144	0.23673	0.91263	0.24121
N	(8b)	0.26927	0.25621	0.49970	0.26769	0.25564	0.49988	0.26505	0.25467	0.50006
W	(4a)	0	0.16653	0.45415	0	0.16646	0.45246	0	0.16633	0.45091
W	(4a)	0	0.67204	0.63491	0	0.67357	0.63480	0	0.67492	0.63482
W	(4a)	0	0.16619	0.84032	0	0.16620	0.83625	0	0.16607	0.83222
W	(8b)	0.24234	0.08637	0.13485	0.23994	0.08717	0.13477	0.23802	0.08794	0.13484

Structure 34: N_8W_5 in the δ_H^{III} structure of Khitrova and Pinsker,[37] constructing a $2 \times 2 \times 1$ supercell of the parent structure (#58 and then removing three tungsten atoms from each of the $z = 0$ and the $z = 1/2$ tungsten (2a) sites, leaving two atoms which are stacked on top of one another.

Space Group		$P6_3/mmc - D_{6h}^4$ (#194)			Pearson Symbol			$oC52$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		5.71061Å	5.71061Å	10.40780Å	5.79250Å	5.79250Å	10.57498Å	5.91055Å	5.91055Å	10.72291Å
α , β , γ		90°	90°	120°	90°	90°	120°	90°	90°	120°
Wyckoff Positions:										
N	(4f)	1/3	2/3	0.63561	1/3	2/3	0.63616	1/3	2/3	0.63606
N	(12k)	0.15969	0.31938	0.12670	0.15896	0.31793	0.12707	0.15835	0.31670	0.12725
W	(2a)	0	0	0	0	0	0	0	0	0
W	(2b)	0	0	1/4	0	0	1/4	0	0	1/4
W	(6h)	0.50271	0.49729	1/4	0.50332	0.49668	1/4	0.50386	0.49614	1/4

7. N_3W_2 structures (x = 0.400)

Structure 35: N_3W_2 structure derived from the r-W_2N_3 structure of WYL+[33] by removing selected tungsten atoms, as described in the text. We use the freedom allowed by this space group to arbitrarily set the position of one of the W (2a) atoms to the origin. This is the lowest energy structure structure r-W_2N_3-like structure we have found.

Space Group		$Cm - C_s^3$ (#8)			Pearson Symbol			$mC20$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		4.96842Å	8.54709Å	5.29894Å	5.03539Å	8.66590Å	5.37753Å	5.13169Å	8.83574Å	5.48077Å
α , β , γ		90°	108.36023°	90°	90°	108.35442°	90°	90°	108.42204°	90°
Wyckoff Positions:										
N	(2a)	0.41209	0	0.26961	0.41217	0	0.27052	0.41100	0	0.26858
N	(2a)	0.59956	0	0.77297	0.60103	0	0.77281	0.60381	0	0.76930
N	(4b)	0.43004	0.34163	0.27194	0.43099	0.34196	0.27285	0.43137	0.34255	0.27118
N	(4b)	0.58810	0.33171	0.77540	0.58740	0.33266	0.77536	0.58489	0.33461	0.77229
W	(2a)	0	0	0	0	0	0	0	0	0
W	(2a)	0.18522	0	0.53915	0.18566	0	0.53898	0.18698	0	0.53770
W	(4b)	0.17041	0.33161	0.51418	0.17078	0.33156	0.51438	0.16956	0.33115	0.51024

Structure 36: N_3W_2 structure derived from the r-W_2N_3 structure of WYL+[33] by removing selected tungsten atoms, as described in the text. This structure is nearly degenerate with Structure 35.

Space Group		$P3_1 - C_3^2$ (#144)			Pearson Symbol			$hP30$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		4.95098Å	4.95098Å	15.09115Å	5.01872Å	5.01872Å	15.31563Å	5.11649Å	5.11649Å	15.60545Å
α , β , γ		90°	90°	120°	90°	90°	120°	90°	90°	120°
Wyckoff Positions:										
N	(3a)	0.89091	0.79421	0.58136	0.89078	0.79490	0.58113	0.89035	0.79659	0.58086
N	(3a)	0.56726	0.11224	0.58190	0.56769	0.11224	0.58171	0.56829	0.11291	0.58156
N	(3a)	0.20734	0.42874	0.58129	0.20655	0.42808	0.58106	0.20487	0.42751	0.58080
N	(3a)	0.89282	0.77556	0.41339	0.89447	0.77753	0.41350	0.89852	0.78203	0.41372
N	(3a)	0.54863	0.11174	0.41422	0.54742	0.11174	0.41437	0.54409	0.11231	0.41473
N	(3a)	0.22879	0.44801	0.41343	0.22847	0.44611	0.41355	0.22859	0.44281	0.41374
W	(3a)	0.88790	0.77584	0.00523	0.88747	0.77529	0.00532	0.88699	0.77417	0.00449
W	(3a)	0.88839	0.77289	0.82560	0.88842	0.77261	0.82574	0.88783	0.77054	0.82534
W	(3a)	0.55111	0.11042	0.83378	0.55098	0.11021	0.83381	0.54951	0.10918	0.83437
W	(3a)	0.22537	0.44734	0.83379	0.22546	0.44720	0.83382	0.22571	0.44700	0.83439

Structure 37: N_3W_2 derived from Structure 11 by tripling the size of the unit cell in the basal plane and removing 2/3 of the tungsten atoms in one of the layers.

Space Group		$P\bar{6}2m - D^3_{3h}$ (#189)			Pearson Symbol			$hP10$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		4.89169Å	4.89169Å	5.30982Å	4.96204Å	4.96204Å	5.38094Å	5.06203Å	5.06203Å	5.47510Å
α , β , γ		90°	90°	120°	90°	90°	120°	90°	90°	120°
Wyckoff Positions:										
N	(6i)	0.68146	0	0.74213	0.68223	0	0.74187	0.68396	0	0.74103
W	(1a)	0	0	0	0	0	0	0	0	0
W	(1b)	0	0	1/2	0	0	1/2	0	0	1/2
W	(2d)	1/3	2/3	1/2	1/3	2/3	1/2	1/3	2/3	1/2

Structure 38: N_3W_2 derived from the NaCl structure by constructing a hexagonal supercell and removing 2/3 of the W atoms in one of the resulting (0001) planes.

Space Group		$C2/m - C^3_{2h}$ (#12)			Pearson Symbol			$mC20$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		5.05162Å	8.86240Å	4.99501Å	5.11511Å	8.98033Å	5.07770Å	5.21590Å	9.17445Å	5.16762Å
α , β , γ		90°	107.89598°	90°	90°	107.85285°	90°	90°	107.57484°	90°
Wyckoff Positions:										
N	(4i)	0.23179	0	0.72319	0.23167	0	0.72265	0.22832	0	0.71823
N	(8j)	0.25368	0.16349	0.23095	0.25336	0.16289	0.23174	0.25293	0.16091	0.23261
W	(2a)	0	0	0	0	0	0	0	0	0
W	(2d)	0	1/2	1/2	0	1/2	1/2	0	1/2	1/2
W	(4h)	0	0.18914	1/2	0	0.18980	1/2	0	0.19222	1/2

Structure 39: N_3W_2 structure derived from the r-W_2N_3 structure of WYL+[33] by removing selected tungsten atoms, as described in the text.

Space Group		$P3_1 - C_3^2$ (#144)			Pearson Symbol			$hP90$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		8.61587Å	8.61587Å	15.34986Å	8.73550Å	8.73550Å	15.65447Å	8.91347Å	8.91347Å	16.01854Å
α , β , γ		90°	90°	120°	90°	90°	120°	90°	90°	120°
Wyckoff Positions:										
N	(3a)	0.34410	0.11592	0.42008	0.34501	0.11859	0.41982	0.35158	0.12767	0.42010
N	(3a)	0.55728	0.23015	0.74863	0.55487	0.22701	0.74893	0.54041	0.22271	0.74978
N	(3a)	0.44807	0.32869	0.08558	0.45072	0.33020	0.08544	0.45633	0.32768	0.08539
N	(3a)	0.33498	0.44910	0.42475	0.33538	0.45144	0.42640	0.34242	0.46292	0.42593
N	(3a)	0.55542	0.55236	0.75179	0.55218	0.54962	0.75185	0.53727	0.54107	0.75248
N	(3a)	0.44685	0.66507	0.09249	0.44830	0.66545	0.09342	0.45377	0.66053	0.09501
N	(3a)	0.99800	0.11664	0.41413	0.99740	0.11904	0.41375	0.00363	0.13008	0.41415
N	(3a)	0.22810	0.22738	0.75199	0.22674	0.22504	0.75184	0.21467	0.22043	0.75295
N	(3a)	0.11422	0.33364	0.09121	0.11613	0.33451	0.09270	0.12079	0.32756	0.09322
N	(3a)	0.33275	0.11435	0.58618	0.33348	0.11721	0.58547	0.34339	0.13355	0.58410
N	(3a)	0.55243	0.21880	0.92043	0.55086	0.21845	0.92147	0.53880	0.21690	0.92443
N	(3a)	0.44206	0.32879	0.25511	0.44469	0.32838	0.25434	0.45179	0.32078	0.25317
N	(3a)	0.33477	0.44602	0.58527	0.33441	0.44560	0.58599	0.34300	0.45302	0.58458
N	(3a)	0.55435	0.55815	0.92159	0.55414	0.55546	0.92105	0.54676	0.55291	0.92148
N	(3a)	0.44584	0.66514	0.25168	0.44868	0.66587	0.25128	0.45377	0.65990	0.25147
N	(3a)	0.00367	0.11055	0.57373	0.00284	0.11280	0.57208	0.00835	0.12461	0.57030
N	(3a)	0.21790	0.21966	0.91912	0.21581	0.21710	0.91860	0.20303	0.20914	0.91935
N	(3a)	0.11014	0.33041	0.25198	0.11154	0.32909	0.25245	0.11535	0.32250	0.25167
W	(3a)	0.30172	0.09346	0.99182	0.29797	0.09144	0.99010	0.28682	0.08491	0.98591
W	(3a)	0.52753	0.20398	0.32962	0.52404	0.20226	0.32975	0.52035	0.19138	0.32980
W	(3a)	0.40781	0.32086	0.66136	0.40261	0.31842	0.66199	0.38647	0.31656	0.66611
W	(3a)	0.33102	0.10764	0.17171	0.33398	0.10834	0.17057	0.33921	0.10225	0.16879
W	(3a)	0.56107	0.22583	0.50479	0.56146	0.22849	0.50433	0.56864	0.24171	0.50389
W	(3a)	0.44605	0.33535	0.83714	0.44484	0.33324	0.83673	0.43370	0.32872	0.83840
W	(3a)	0.33601	0.44812	0.17190	0.33844	0.44924	0.17234	0.34442	0.44440	0.17309
W	(3a)	0.55528	0.56029	0.49221	0.55493	0.56177	0.49303	0.55924	0.57182	0.49029
W	(3a)	0.43575	0.66354	0.83820	0.43348	0.66141	0.83889	0.42207	0.65662	0.83953
W	(3a)	0.00284	0.10984	0.16496	0.00551	0.11017	0.16476	0.01175	0.10276	0.16380
W	(3a)	0.22270	0.22551	0.49848	0.22254	0.22757	0.49861	0.22931	0.23829	0.49737
W	(3a)	0.11224	0.34046	0.84008	0.11090	0.33958	0.84001	0.10035	0.33644	0.84145

Structure 40: N_3W_2 structure derived from the r-W_2N_3 structure of WYL+[33] by removing selected tungsten atoms, as described in the text.

Space Group		$Cm - C_s^3$ (#8)			Pearson Symbol			$mC60$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		14.96460Å	2.86583Å	15.48567Å	15.18062Å	2.90361Å	15.78788Å	15.47017Å	2.96720Å	16.07847Å
α , β , γ		90°	93.77314°	90°	90°	94.18013°	90°	90°	94.38069°	90°
Wyckoff Positions:										
N	(2a)	0.99517	0	0.58094	0.99602	0	0.58107	0.99570	0	0.58082
N	(2a)	0.45314	0	0.24515	0.45302	0	0.24475	0.45413	0	0.24517
N	(2a)	0.55627	0	0.91518	0.55636	0	0.91543	0.55612	0	0.91452
N	(2a)	0.34083	0	0.58051	0.34173	0	0.58033	0.34193	0	0.57921
N	(2a)	0.78645	0	0.24406	0.78678	0	0.24339	0.78743	0	0.24348
N	(2a)	0.89878	0	0.91169	0.89935	0	0.91116	0.89978	0	0.91105
N	(2a)	0.66817	0	0.57503	0.66877	0	0.57338	0.66898	0	0.57461
N	(2a)	0.11076	0	0.24935	0.11015	0	0.24944	0.11087	0	0.24922
N	(2a)	0.23122	0	0.91060	0.23237	0	0.90985	0.23222	0	0.90937
N	(2a)	0.99412	0	0.41214	0.99399	0	0.41233	0.99626	0	0.41325
N	(2a)	0.44116	0	0.07843	0.44103	0	0.07790	0.44276	0	0.07798
N	(2a)	0.55608	0	0.74861	0.55553	0	0.74964	0.55374	0	0.74927
N	(2a)	0.32257	0	0.42094	0.32266	0	0.42209	0.32209	0	0.42176
N	(2a)	0.77434	0	0.08821	0.77357	0	0.08881	0.77391	0	0.08921
N	(2a)	0.88585	0	0.74506	0.88667	0	0.74454	0.88759	0	0.74392
N	(2a)	0.66144	0	0.41719	0.66062	0	0.41667	0.65863	0	0.41810
N	(2a)	0.11060	0	0.08325	0.10917	0	0.08421	0.10769	0	0.08440
N	(2a)	0.21995	0	0.75420	0.21993	0	0.75471	0.21962	0	0.75449
W	(2a)	0.00066	0	0.00267	0.00034	0	0.00274	0.09985	0	0.00183
W	(2a)	0.44498	0	0.66932	0.44569	0	0.66944	0.44506	0	0.66861
W	(2a)	0.55574	0	0.33774	0.55499	0	0.33766	0.55562	0	0.33703
W	(2a)	0.00105	0	0.82764	0.00108	0	0.82826	0.00103	0	0.82815
W	(2a)	0.43563	0	0.49117	0.43570	0	0.49189	0.43500	0	0.49089
W	(2a)	0.55575	0	0.16202	0.55494	0	0.16250	0.55564	0	0.16293
W	(2a)	0.33055	0	0.83238	0.33040	0	0.83212	0.32886	0	0.83271
W	(2a)	0.77552	0	0.49883	0.77588	0	0.49851	0.77580	0	0.49778
W	(2a)	0.88580	0	0.16572	0.88486	0	0.16561	0.88420	0	0.16681
W	(2a)	0.67165	0	0.83262	0.67244	0	0.83269	0.67223	0	0.83178
W	(2a)	0.10936	0	0.50459	0.10964	0	0.50412	0.11040	0	0.50745
W	(2a)	0.22639	0	0.16676	0.22634	0	0.16676	0.22684	0	0.16618

Structure 41: N_3W_2 in the lower symmetry form of two possible structures for the mineral Bixbyite.[39]

Space Group		$I2_13 - T^5$ (#199)			Pearson Symbol			$cI80$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		9.45320Å	9.45320Å	9.45320Å	9.60076Å	9.60076Å	9.60076Å	9.90521Å	9.90521Å	9.90521Å
α , β , γ		90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:										
N	(24c)	0.09352	0.65344	0.40160	0.09486	0.65441	0.40087	0.09447	0.64230	0.36856
N	(24c)	0.36648	0.61279	0.33002	0.37024	0.61222	0.32975	0.36622	0.59398	0.35298
W	(8a)	0.23169	0.76831	0.26831	0.23475	0.76525	0.26525	0.23442	0.76558	0.26558
W	(12b)	0	1/4	0.47049	0	1/4	0.46694	0	1/4	0.48663
W	(12b)	0	1/4	0.92970	0	1/4	0.93017	0	1/4	0.99062

Structure 42: N_3W_2 in the higher symmetry form of two possible structures for the mineral Bixbyite.[40]

Space Group		$Ia\bar{3} - T_h^7$ (#206)			Pearson Symbol			$cI80$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		9.49336Å	9.49336Å	9.49336Å	9.63327Å	9.63327Å	9.63327Å	9.83654Å	9.83654Å	9.83654Å
α , β , γ		90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:										
N	(48e)	0.11072	0.89898	0.16523	0.11017	0.89815	0.16511	0.11105	0.89584	0.16358
W	(8b)	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4
W	(24d)	0.44016	0	1/4	0.43958	0	1/4	0.44515	0	1/4

Structure 43: N_3W_2 constructed from the δ_H^I NW structure of Khitrova and Pinsker,[37] fully filling all sites and reversing the N and W occupancies on each site. This is the h-W_2N_3 structure considered by WYL+,[33] and is the reverse of Structure 80.

Space Group		$P6_3/mmc - D_{6h}^4$ (#194)			Pearson Symbol			$hP10$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		2.87929Å	2.87929Å	15.18835Å	2.91812Å	2.91812Å	16.75176Å	2.98189Å	2.98189Å	15.90534Å
α , β , γ		90°	90°	120°	90°	90°	120°	90°	90°	120°
Wyckoff Positions:										
N	(2c)	1/3	2/3	1/4	1/3	2/3	1/4	1/3	2/3	1/4
N	(4f)	1/3	2/3	0.08182	1/3	2/3	0.09546	1/3	2/3	0.08495
W	(4f)	1/3	2/3	0.65477	1/3	2/3	0.66217	1/3	2/3	0.65507

8. N_4W_3 structures (x = 0.42857)

Structure 44: N_4W_3 constructed constructing a $2\times2\times2$ supercell of the WC structure (#61) and removing two nitrogen atoms in the same plane.

Space Group		$Pmm2-C_{2v}^{1}$ (#25)			Pearson Symbol			$oP7$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		2.80932Å	5.45541Å	4.91334Å	2.84553Å	5.53407Å	4.99104Å	2.90562Å	5.64162Å	5.08715Å
α , β , γ		90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:										
N	(2g)	0	0.26552	0.01266	0	0.26613	0.01333	0	0.26782	0.01425
N	(2h)	1/2	0.25079	0.49338	1/2	0.25121	0.49293	1/2	0.25223	0.49256
W	(1a)	0	0	0.31512	0	0	0.31371	0	0	0.31210
W	(1b)	0	1/2	0.33156	0	1/2	0.33136	0	1/2	0.33162
W	(1d)	1/2	1/2	0.84124	1/2	1/2	0.84241	1/2	1/2	0.84267

Structure 45: N_4W_3 constructed by removing four tungsten atoms from a cI64 supercell of the NaCl structure.

Space Group		$Cmmm-D_{2h}^{17}$ (#63)			Pearson Symbol			$oC28$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		8.25439Å	8.60397Å	4.13203Å	8.37442Å	8.76136Å	4.18309Å	8.60115Å	8.98633Å	4.24779Å
α , β , γ		90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:										
N	(4c)	0	0.12632	1/4	0	0.12542	1/4	0	0.12302	1/4
N	(4c)	0	0.63028	1/4	0	0.63202	1/4	0	0.63287	1/4
N	(8g)	0.25697	0.89405	1/4	0.25662	0.89446	1/4	0.25313	0.89560	1/4
W	(4c)	0	0.87414	1/4	0	0.87467	1/4	0	0.87525	1/4
W	(8g)	0.27051	0.14408	1/4	0.27183	0.14520	1/4	0.27590	0.14646	1/4

Structure 46: N_4W_3 constructed by removing two tungsten atoms from a cF64 supercell of the NaCl structure.

Space Group		$Cmmm-D_{2h}^{19}$ (#65)			Pearson Symbol			$oC14$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		8.15313Å	5.99794Å	2.97257Å	8.24882Å	6.10953Å	3.01259Å	8.40782Å	6.19562Å	3.11096Å
α , β , γ		90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:										
N	(4g)	0.26143	0	0	0.26184	0	0	0.26014	0	0
N	(4j)	0	0.25090	1/2	0	0.24913	1/2	0	0.24522	1/2
W	(2a)	0	0	0	0	0	0	0	0	0
W	(4f)	1/4	1/4	1/2	1/4	1/4	1/2	1/4	1/4	1/2

Structure 47: N_4W_3 in the S_3U_4 structure.[41] This is the c-W_3N_4 structure considered by WYL+ and others.[33,42,43]

Space Group		$Pm\bar{3}m - O_h^1$ (#221)			Pearson Symbol			$cP7$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		4.17013Å	4.17013Å	4.17013Å	4.22769Å	4.22769Å	4.22769Å	4.31596Å	4.31596Å	4.31596Å
α , β , γ		90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:										
N	(1a)	0	0	0	0	0	0	0	0	0
N	(3c)	0	1/2	1/2	0	1/2	1/2	0	1/2	1/2
W	(3d)	1/2	0	0	1/2	0	0	1/2	0	0

9. N_6W_5 structures (x = 0.45455)

Structure 48: N_6W_5 structure derived from the r-W_2N_3 structure of WYL+.[33] This is based on Structure 35, reversing the pattern of tungsten atoms and vacancies.

Space Group		$Cm - C_s^3$ (#8)			Pearson Symbol			$mC22$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		4.86659Å	8.44454Å	5.75306Å	4.93311Å	8.56120Å	5.84214Å	5.02889Å	8.72702Å	5.99409Å
α , β , γ		90°	106.45362°	90°	90°	106.43974°	90°	90°	106.40344°	90°
Wyckoff Positions:										
N	(2a)	0.42572	0	0.25792	0.42675	0	0.25900	0.43028	0	0.26180
N	(2a)	0.58257	0	0.73599	0.58235	0	0.73517	0.58057	0	0.73263
N	(4b)	0.07674	0.83417	0.73559	0.07640	0.83410	0.73474	0.07605	0.83330	0.73208
N	(4b)	0.41541	0.33098	0.25793	0.41529	0.33063	0.25891	0.41414	0.32957	0.26143
W	(2a)	0.83746	0	0.50235	0.83750	0	0.50264	0.83817	0	0.50465
W	(4b)	0.49850	0.83336	0.99256	0.49856	0.83336	0.99206	0.49935	0.33349	0.99129
W	(4b)	0.32848	0.83528	0.49178	0.32846	0.83528	0.49189	0.32795	0.33546	0.49168

10. N_7W_6 structures (x = 0.46154)

Structure 49: N_7W_6 structure constructed from a cF64 supercell of the NaCl structure.

Space Group		$Fm\bar{3}m - O_h^5$ (#225)			Pearson Symbol			$cF52$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		8.24485Å	8.24485Å	8.24485Å	8.35636Å	8.35636Å	8.35636Å	8.51771Å	8.51771Å	8.51771Å
α , β , γ		90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:										
N	(4b)	1/2	1/2	1/2	1/2	1/2	1/2	1/2	1/2	1/2
N	(24d)	0	1/4	1/4	0	1/4	1/4	0	1/4	1/4
W	(24e)	0.23122	0	0	0.23068	0	0	0.22977	0	0

11. N_8W_7 structures (x = 0.46667)

Structure 50: N_8W_7 structure constructed from a cF64 supercell of the NaCl structure, removing one tungsten atom.

Space Group		$Fm\bar{3}m - O_h^5$ (#225)			Pearson Symbol			$cF60$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		8.46990Å	8.46990Å	8.46990Å	8.59363Å	8.59363Å	8.59363Å	8.79478Å	8.79478Å	8.79478Å
α , β , γ		90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:										
N	(8c)	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4
N	(24e)	0.25622	0	0	0.25593	0	0	0.25362	0	0
W	(4a)	0	0	0	0	0	0	0	0	0
W	(24d)	0	1/4	1/4	0	1/4	1/4	0	1/4	1/4

Structure 51: N_8W_7 structure constructed from a $2 \times 2 \times 2$ supercell of the tungsten carbide structure (#61), removing one tungsten atom.

Space Group		$P\bar{6}m2 - D_{3h}^1$ (#187)			Pearson Symbol			$hP15$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		5.66164Å	5.66164Å	5.55015Å	5.74123Å	5.74123Å	5.62972Å	5.86240Å	5.86240Å	5.75495Å
α , β , γ		90°	90°	120°	90°	90°	120°	90°	90°	120°
Wyckoff Positions:										
N	(2i)	2/3	1/3	0.24591	2/3	1/3	0.24538	2/3	1/3	0.24478
N	(6n)	0.16684	0.33368	0.25493	0.16683	0.33368	0.25547	0.16764	0.33528	0.25771
W	(1b)	0	0	0	0	0	0	0	0	0
W	(3j)	0.49939	0.99878	0	0.49939	0.99876	0	0.49970	0.99940	0
W	(3k)	0.49638	0.99276	1/2	0.49590	0.99180	1/2	0.49552	0.99104	1/2

12. $N_{13}W_{12}$ structures (x = 0.480)

Structure 52: $N_{13}W_{12}$ structure constructed from a $2 \times 2 \times 2$ supercell of the NbO structure, replacing one of the nitrogen vacancy sites by a nitrogen atom.

Space Group		$Im\bar{3}m - O_h^9$ (#229)			Pearson Symbol			$cI50$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		8.19323Å	8.19323Å	8.19323Å	8.30255Å	8.30255Å	8.30255Å	8.46211Å	8.46211Å	8.46211Å
α , β , γ		90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:										
N	(2a)	0	0	0	0	0	0	0	0	0
N	(24h)	0	0.25094	0.25094	0	0.25090	0.25090	0	0.25070	0.25070
W	(12d)	0	1/2	1/4	0	1/2	1/4	0	1/2	1/4
W	(12e)	0.26125	0	0	0.26217	0	0	0.26499	0	0

13. NW structures (x = 0.500)

Structure 53: NW in the NbO structure.[44] This structure was studied in detail by Liu, Zhou, Gall and Khare[45].

Space Group		$Pm\bar{3}m - O_h^1$ (#221)			Pearson Symbol			$cP6$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		4.07801Å	4.07801Å	4.07801Å	4.13144Å	4.13144Å	4.13144Å	4.20844Å	4.20844Å	4.20844Å
α , β , γ		90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:										
N	(3d)	1/2	0	0	1/2	0	0	1/2	0	0
W	(3c)	0	1/2	1/2	0	1/2	1/2	0	1/2	1/2

Structure 54: NW constructed by placing N and W vacancies on a 16 atom body-centered tetragonal supercell of the NaCl structure.

Space Group		$I4mm - C_{4v}^9$ (#107)			Pearson Symbol			$tI24$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		4.10200Å	4.10200Å	16.26180Å	4.15925Å	4.15925Å	16.47511Å	4.23932Å	4.23932Å	16.83746Å
α , β , γ		90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:										
N	(2a)	0	0	0.25063	0	0	0.25072	0	0	0.25101
N	(2a)	0	0	0.49837	0	0	0.49951	0	0	0.50379
N	(4b)	0	1/2	0.12467	0	1/2	0.12407	0	1/2	0.12202
N	(4b)	0	1/2	0.37408	0	1/2	0.37401	0	1/2	0.37361
W	(2a)	0	0	0.62892	0	0	0.63043	0	0	0.63508
W	(2a)	0	0	0.88054	0	0	0.88116	0	0	0.88287
W	(4b)	0	1/2	0.24872	0	1/2	0.24825	0	1/2	0.24710
W	(4b)	0	1/2	0.49830	0	1/2	0.49776	0	1/2	0.49590

Structure 55: NW constructed by placing vacancies on an 8 atom body-centered tetragonal supercell of the NaCl structure.

Space Group		$I4mm - C_{4v}^9$ (#107)			Pearson Symbol			$tI24$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		4.12998Å	4.12998Å	8.13034Å	4.18771Å	4.18771Å	8.24079Å	4.23955Å	4.23955Å	8.38322Å
α , β , γ		90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:										
N	(2a)	0	0	0.99315	0	0	0.99220	0	0	0.98872
N	(4b)	0	1/2	0.25443	0	1/2	0.25473	0	1/2	0.25654
W	(2a)	0	0	0.72998	0	0	0.72855	0	0	0.72503
W	(4b)	0	1/2	0.00901	0	1/2	0.00989	0	1/2	0.01159

Structure 56: NW by adding one nitrogen and one tungsten atom to a 24 atom body-centered supercell of the NbO structure (#53). This is the highest symmetry crystal that can be constructed in this fashion.

Space Group		$R\bar{3}m - D^5_{3d}$ (#166)			Pearson Symbol			$hR78$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		11.70769Å	11.70769Å	7.12262Å	11.86214Å	11.86214Å	7.22654Å	12.09841Å	12.09841Å	7.38466Å
α , β , γ		90°	90°	120°	90°	90°	120°	90°	90°	120°
Wyckoff Positions:										
N	(3a)	0	0	0	0	0	0	0	0	0
N	(18f)	0.25164	0	0	0.25152	0	0	0.25091	0	0
N	(18h)	-0.08700	0.08700	0.32510	-0.08686	0.08686	0.32458	-0.08597	0.08597	0.32430
W	(3b)	0	0	1/2	0	0	1/2	0	0	1/2
W	(18g)	0.25165	0	1/2	0.25164	0	1/2	0.25204	0	1/2
W	(18h)	0.08888	-0.08888	0.16984	0.08954	-0.08954	0.17103	0.09155	-0.09155	0.17457

Structure 57: NW by removing one nitrogen and one tungsten atom from a cF64 supercell of the NaCl structure (#67), or, alternatively, by adding one nitrogen and one tungsten atom to a 12 atom face-centered supercell of the NbO structure (#53). This is the highest symmetry crystal that can be constructed in this fashion.

Space Group		$F\bar{4}3m - T^2_d$ (#216)			Pearson Symbol			$cF56$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		8.37316Å	8.37316Å	8.37316Å	8.49476Å	8.49476Å	8.49476Å	8.68207Å	8.68207Å	8.68207Å
α , β , γ		90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:										
N	(4b)	1/2	1/2	1/2	1/2	1/2	1/2	1/2	1/2	1/2
N	(24g)	0.49049	1/4	1/4	0.40973	1/4	1/4	0.49245	1/4	1/4
W	(4d)	3/4	3/4	3/4	3/4	3/4	3/4	3/4	3/4	3/4
W	(24f)	0.23053	0	0	0.22964	0	0	0.22804	0	0

Structure 58: NW in the parent of the δ^{III}_H structure of Khitrova and Pinsker,[37] with the tungsten (2a) site fully occupied. The stacking is ABABACAC, with the tungsten atoms on the A sites. Compare this to the AsNi structure (#59), where the stacking is ABAC.

Space Group		$P6_3/mmc - D^4_{6h}$ (#194)			Pearson Symbol			$hP8$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		2.82708Å	2.82708Å	11.44132Å	2.86485Å	2.86485Å	11.63195Å	2.92335Å	2.92335Å	11.93905Å
α , β , γ		90°	90°	120°	90°	90°	120°	90°	90°	120°
Wyckoff Positions:										
N	(4f)	1/3	2/3	0.12966	1/3	2/3	0.13024	1/3	2/3	0.13162
W	(2a)	0	0	0	0	0	0	0	0	0
W	(2b)	0	0	1/2	0	0	1/2	0	0	1/2

Structure 59: NW in the AsNi structure.[46] with nitrogen on the As (2c) site. Compare the stacking here to the parent of the δ_H^{III} structure (#58). Kroll, Schröter and Peters[29] assume that this is the ground state of tungsten nitride. The reversed structure, with tungsten on the As site, is much higher in energy and is not considered here.

Space Group	$P6_3/mmc - D_{6h}^4$ (#194)			Pearson Symbol			$hP4$		
Functional	LDA			PBE			vdW-DF2		
a , b , c	2.81931Å	2.81931Å	5.72655Å	2.85823Å	2.85823Å	5.81546Å	2.91989Å	2.91989Å	5.95435Å
α , β , γ	90°	90°	120°	90°	90°	120°	90°	90°	120°
Wyckoff Positions:									
N (2c)	1/3	2/3	1/4	1/3	2/3	1/4	1/3	2/3	1/4
W (2a)	0	0	0	0	0	0	0	0	0

Structure 60: NW by removing on nitrogen and one tungsten atom from a 24 atom body-centered supercell of the NbO structure (#53).

Space Group	$C2/m - C_{2h}^3$ (#12)			Pearson Symbol			$mC44$		
Functional	LDA			PBE			vdW-DF2		
a , b , c	7.97757Å	11.51413Å	7.02914Å	8.06566Å	11.70348Å	7.12924Å	8.19150Å	11.95035Å	7.26586Å
α , β , γ	90°	55.74886°	90°	90°	55.88138°	90°	90°	56.02006°	90°
Wyckoff Positions:									
N (2a)	0	0	0	0	0	0	0	0	0
N (4f)	1/4	1/4	1/2	1/4	1/4	1/2	1/4	1/4	1/2
N (8j)	0.37023	0.37865	-0.24593	0.36976	0.37808	-0.24526	0.36927	0.37768	-0.24458
N (8j)	0.37560	0.12361	-0.24985	0.37568	0.12339	-0.24991	0.37583	0.12319	-0.25005
W (2d)	0	1/2	1/2	0	1/2	1/2	0	1/2	1/2
W (4e)	1/4	1/4	0	1/4	1/4	0	1/4	1/4	0
W (8j)	0.11534	0.12632	-0.24330	0.11451	0.12650	-0.24161	0.11354	0.12640	-0.24057
W (8j)	0.13360	0.36960	-0.25398	0.13413	0.36821	-0.25467	0.13558	0.36761	-0.25574

Structure 61: NW in the tungsten carbide (WC) structure. This is the δ-WN structure studied by WYL+[33] and was earlier studied computationally by Suetin, Shein, and Ivanovskii.[47]

Space Group	$P\bar{6}m2 - D_{3h}^1$ (#187)			Pearson Symbol			$hP2$		
Functional	LDA			PBE			vdW-DF2		
a , b , c	2.83505Å	2.83505Å	2.86729Å	2.87255Å	2.87255Å	2.91440Å	2.93274Å	2.93274Å	2.98489Å
α , β , γ	90°	90°	120°	90°	90°	120°	90°	90°	120°
Wyckoff Positions:									
N (1a)	0	0	0	0	0	0	0	0	0
W (1d)	1/3	2/3	1/2	1/3	2/3	1/2	1/3	2/3	1/2

Structure 62: NW in the Wurtzite structure. We arbitrarily set the z coordinate of the Nitrogen atom to zero.

Space Group	$P6_3mc - C_{6v}^4$ (#186)			Pearson Symbol			$hP4$		
Functional	LDA			PBE			vdW-DF2		
a , b , c	2.87871Å	2.87871Å	6.38093Å	2.92216Å	2.92216Å	6.46259Å	2.98529Å	2.98529Å	6.58033Å
α , β , γ	90°	90°	120°	90°	90°	120°	90°	90°	120°
Wyckoff Positions:									
N (2b)	1/3	2/3	0.00000	1/3	2/3	0.00000	1/3	2/3	0.00000
W (2b)	1/3	2/3	0.31040	1/3	2/3	0.31051	1/3	2/3	0.30929

Structure 63: NW in the r-W_2N_3 structure proposed by WYL+.[33] In this base structure both W sites are fully occupied. Note that the original paper gives the space group as $R3$, but the coordinates are consistent with $R3m$, which we use here. The first W atom position was arbitrarily set at the origin.

Space Group		$R3m - C_{3v}^5$ (#160)			Pearson Symbol			$hR12$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		2.82513Å	2.82513Å	17.19116Å	2.86376Å	2.86376Å	17.49094Å	2.91952Å	2.91952Å	18.02952Å
α , β , γ		90°	90°	120°	90°	90°	120°	90°	90°	120°
Wyckoff Positions:										
N	(3a)	0	0	0.25469	0	0	0.25310	0	0	0.25559
N	(3a)	0	0	0.41366	0	0	0.41112	0	0	0.41148
W	(3a)	0	0	0	0	0	0	0	0	0
W	(3a)	0	0	0.83518	0	0	0.83564	0	0	0.83639

Structure 64: NW in the δ_H^{IV} structure of Khitrova and Pinsker, with all sites fully occupied.[37] Although they list the space group as $P6_3$ rather than $P6_3mc$, for these Wyckoff positions the space groups are identical. We choose the higher symmetry of the $P6_3mc$ space group. Also note that Khitrova and Pinsker set the z variable for both nitrogen sites to 1/4. This is not supported by the calculation.

Space Group		$P^-3mc - C_{6v}^4$ (#186)			Pearson Symbol			$hP8$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		3.16439Å	3.16439Å	12.94609Å	3.19679Å	3.19679Å	15.04969Å	3.33219Å	3.33219Å	13.37224Å
α , β , γ		90°	90°	120°	90°	90°	120°	90°	90°	120°
Wyckoff Positions:										
N	(2a)	0	0	0.22697	0	0	0.24429	0	0	0.23626
N	(2b)	1/3	2/3	0.52434	1/3	2/3	0.50577	1/3	2/3	0.51455
W	(2b)	1/3	2/3	-0.03058	1/3	2/3	-0.04216	1/3	2/3	-0.03175
W	(2b)	1/3	2/3	0.77927	1/3	2/3	0.79209	1/3	2/3	0.780943

Structure 65: NW in the zincblende structure.[48] This is the c-BN structure in WYL+.[33]

Space Group		$F\bar{4}3m - T_d^2$ (#216)			Pearson Symbol			$cF8$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		4.60727Å	4.60727Å	4.60727Å	4.67252Å	4.67252Å	4.67252Å	4.77342Å	4.77342Å	4.77342Å
α , β , γ		90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:										
N	(4a)	0	0	0	0	0	0	0	0	0
W	(4c)	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4

Structure 66: NW constructed by removing on nitrogen and one tungsten atom from a 12 atom face-centered cubic supercell of the NbO structure (#53).

Space Group		$I\bar{4}m2 - D_{2d}^{9}$ (#119)			Pearson Symbol			$tI20$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		5.77619Å	5.77619Å	7.79654Å	5.89761Å	5.89761Å	7.86723Å	6.07122Å	6.07122Å	7.95598Å
α , β , γ		90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:										
N	(2a)	0	0	0	0	0	0	0	0	0
N	(8h)	0.24854	0.74854	1/4	0.24969	0.74969	1/4	0.25141	0.75141	1/4
W	(2d)	0	1/2	3/4	0	1/2	3/4	0	1/2	3/4
W	(8g)	0.24808	0.24808	0	0.24589	0.24589	0	0.24284	0.24284	0

Structure 67: NW in the NaCl structure.

Space Group		$Fm\bar{3}m - O_{h}^{5}$ (#225)			Pearson Symbol			$cF8$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		4.30140Å	4.30140Å	4.30140Å	4.36588Å	4.36588Å	4.36588Å	4.47404Å	4.47404Å	4.47404Å
α , β , γ		90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:										
N	(4a)	0	0	0	0	0	0	0	0	0
W	(4b)	1/2	1/2	1/2	1/2	1/2	1/2	1/2	1/2	1/2

14. $N_{12}W_{13}$ structures (x = 0.520)

Structure 68: $N_{12}W_{13}$ structure constructed from a cI64 supercell of the NaCl structure. This is the reverse of Structure 52.

Space Group		$Im\bar{3}m - O_{h}^{9}$ (#229)			Pearson Symbol			$cI50$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		8.22119Å	8.22119Å	8.22119Å	8.33189Å	8.33189Å	8.33189Å	8.49968Å	8.49968Å	8.49968Å
α , β , γ		90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:										
N	(12d)	0	1/2	1/4	0	1/2	1/4	0	1/2	1/4
N	(12e)	0.26197	0	0	0.26195	0	0	0.26071	0	0
W	(2a)	0	0	0	0	0	0	0	0	0
W	(24h)	0	0.24713	0.24713	0	0.24703	0.24703	0	0.24651	0.24651

15. $N_{11}W_{12}$ structures (x = 0.52174)

Structure 69: $N_{11}W_{12}$ structure constructed from a cI64 supercell of the NbO structure (#53), with one nitrogen atom removed.

Space Group		$I4/mmm - D_{4h}^{17}$ (#139)			Pearson Symbol			$tI46$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		8.15793Å	8.15793Å	8.11911Å	8.27186Å	8.27186Å	8.21962Å	8.43054Å	8.43054Å	8.36803Å
α , β , γ		90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:										
N	(2a)	0	0	0	0	0	0	0	0	0
N	(4c)	0	1/2	0	0	1/2	0	0	1/2	0
N	(16n)	0	0.24938	0.25095	0	0.24928	0.25105	0	0.24905	0.25123
W	(8f)	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4
W	(8i)	0.24874	0	0	0.24842	0	0	0.24822	0	0
W	(8j)	0.24453	1/2	0	0.24361	1/2	0	0.24388	1/2	0

16. N_7W_8 structures (0.53333)

Structure 70: N_7W_8 structure constructed from a $2 \times 2 \times 2$ supercell of the tungsten carbide structure (#61), removing one nitrogen atom. This is the reverse of structure 51.

Space Group		$P\bar{6}m2 - D_{3h}^{1}$ (#187)			Pearson Symbol			$hP15$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		5.67605Å	5.67605Å	5.63159Å	5.75661Å	5.75661Å	5.71189Å	5.88902Å	5.88902Å	5.82678Å
α , β , γ		90°	90°	120°	90°	90°	120°	90°	90°	120°
Wyckoff Positions:										
N	(1b)	0	0	0	0	0	0	0	0	0
N	(3j)	0.49759	0.99518	0	0.49754	0.99508	0	0.49737	0.49474	0
N	(3k)	0.50354	0.00708	1/2	0.50363	0.00726	1/2	0.50437	0.00874	1/2
W	(2i)	2/3	1/3	0.24894	2/3	1/3	0.24906	2/3	1/3	0.24904
W	(6n)	0.16455	0.32911	0.24689	0.16406	0.32812	0.24627	0.16287	0.32574	0.24486

Structure 71: N_7W_8 structure constructed from a cF64 supercell of the NaCl structure, removing one nitrogen atom.

Space Group		$Fm\bar{3}m - O_h^5$ (#225)			Pearson Symbol			$cF60$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		8.53345Å	8.53345Å	8.53345Å	8.66268Å	8.66268Å	8.66268Å	8.86902Å	8.86902Å	8.86902Å
α , β , γ		90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:										
N	(4a)	0	0	0	0	0	0	0	0	0
N	(24d)	0	1/4	1/4	0	1/4	1/4	0	1/4	1/4
W	(8c)	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4
W	(24e)	0.27080	0	0	0.27197	0	0	0.27402	0	0

17. N_6W_7 structures (0.53846)

Structure 72: N_6W_7 structure constructed from a cF64 supercell of the NaCl structure. This is the reverse of Structure 49.

Space Group	$Fm\bar{3}m - O_h^5$ (#225)			Pearson Symbol			$cF52$		
Functional	LDA			PBE			vdW-DF2		
a , b , c	8.29664Å	8.29664Å	8.29664Å	8.41188Å	8.41188Å	8.41188Å	8.58961Å	8.58961Å	8.58961Å
α , β , γ	90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:									
N (24e)	0.24097	0	0	0.24108	0	0	0.24233	0	0
W (4b)	1/2	1/2	1/2	1/2	1/2	1/2	1/2	1/2	1/2
W (24d)	0	1/4	1/4	0	1/4	1/4	0	1/4	1/4

Structure 73: N_6W_7 approximation to the δ_R^{VI} structure of Khitrova and Pinsker,[37] removing two tungsten atoms from the (6c) site of the fully occupied structure (#81).

Space Group	$P\bar{3}m1 - D_{3d}^3$ (#164)			Pearson Symbol			$hP13$		
Functional	LDA			PBE			vdW-DF2		
a , b , c	2.82543Å	2.82543Å	20.31923Å	2.86551Å	2.86551Å	20.61325Å	2.92660Å	2.92660Å	21.04110Å
α , β , γ	90°	90°	120°	90°	90°	120°	90°	90°	120°
Wyckoff Positions:									
N (2c)	0	0	0.24017	0	0	0.24036	0	0	0.24050
N (2d)	1/3	2/3	-0.07193	1/3	2/3	-0.07205	1/3	2/3	-0.07219
N (2d)	1/3	2/3	0.37713	1/3	2/3	0.37735	1/3	2/3	0.37758
W (1a)	0	0	0	0	0	0	0	0	0
W (2c)	0	0	0.14197	0	0	0.14220	0	0	0.14308
W (2d)	1/3	2/3	0.55731	1/3	2/3	0.55722	1/3	2/3	0.55676
W (2d)	1/3	2/3	0.69710	1/3	2/3	0.69723	1/3	2/3	0.69738

18. N_4W_5 structures (x = 0.55556)

Structure 74: N_4W_5 constructed from the δ_H^I structure of Khitrova and Pinsker,[37] removing one of the (4f) W atoms. See Structure 80 for the fully-occupied structure. We arbitrarily set the first nitrogen atom at the origin.

Space Group	$P3m1 - C_{3v}^1$ (#156)			Pearson Symbol			$hP9$		
Functional	LDA			PBE			vdW-DF2		
a , b , c	2.84311Å	2.84311Å	14.01172Å	2.88269Å	2.88269Å	14.21584Å	2.94619Å	2.94619Å	14.49717Å
α , β , γ	90°	90°	120°	90°	90°	120°	90°	90°	120°
Wyckoff Positions:									
N (1a)	0	0	0	0	0	0	0	0	0
N (1a)	0	0	0.81188	0	0	0.81288	0	0	0.81481
N (1b)	1/3	2/3	0.24893	1/3	2/3	0.24968	1/3	2/3	0.25068
N (1b)	1/3	2/3	0.44910	1/3	2/3	0.44901	1/3	2/3	0.44766
W (1a)	0	0	0.14555	0	0	0.14563	0	0	0.14482
W (1a)	0	0	0.34792	0	0	0.35026	0	0	0.35062
W (1a)	0	0	0.55165	0	0	0.55264	0	0	0.55469
W (1b)	1/3	2/3	-0.08904	1/3	2/3	-0.08863	1/3	2/3	-0.08818
W (1b)	1/3	2/3	0.71024	1/3	2/3	0.71034	1/3	2/3	0.70941

19. N_3W_4 structures (x = 0.57143)

Structure 75: N_3W_4 constructed by adding a nitrogen atom to the MoS_2 structure (#89).

Space Group		$P\bar{3}m1 - D_{3d}^3$ (#164)			Pearson Symbol			$hP7$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		2.81594Å	2.81594Å	10.92596Å	2.85399Å	2.85399Å	11.10251Å	2.91042Å	2.91042Å	11.38128Å
α , β , γ		90°	90°	120°	90°	90°	120°	90°	90°	120°
Wyckoff Positions:										
N	(1a)	0	0	0	0	0	0	0	0	0
N	(2d)	1/3	2/3	0.73127	1/3	2/3	0.73068	1/3	2/3	0.72942
W	(2d)	1/3	2/3	0.13324	1/3	2/3	0.13356	1/3	2/3	0.13415
W	(2d)	1/3	2/3	0.39370	1/3	2/3	0.39405	1/3	2/3	0.39520

Structure 76: N_3W_4 constructed by removing two nitrogen atoms from a cF64 supercell of the NaCl structure. This is the reverse of structure #46.

Space Group		$Cmmm - D_{2h}^{19}$ (#65)			Pearson Symbol			$oC14$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		8.45241Å	6.06386Å	2.94913Å	8.57987Å	6.15299Å	2.99378Å	8.78354Å	6.29248Å	3.06078Å
α , β , γ		90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:										
N	(2a)	0	0	0	0	0	0	0	0	0
N	(4f)	1/4	1/4	1/2	1/4	1/4	1/2	1/4	1/4	1/2
W	(4g)	0.27363	0	0	0.27465	0	0	0.27703	0	0
W	(4j)	0	0.28070	1/2	0	0.28234	1/2	0	0.28464	1/2

Structure 77: N_3W_4 constructed by removing four tungsten atoms from a cI64 supercell of the NaCl structure. This is the reverse of structure #45.

Space Group		$Cmcm - D_{2h}^{17}$ (#63)			Pearson Symbol			$oC28$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		8.47033Å	8.56238Å	4.17308Å	8.62957Å	8.69150Å	4.22634Å	8.89047Å	8.91381Å	4.30048Å
α , β , γ		90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:										
N	(4c)	0	0.88342	1/4	0	0.88054	1/4	0	0.87543	1/4
N	(8g)	0.25033	0.14516	1/4	0.24935	0.14373	1/4	0.24699	0.14253	1/4
W	(4c)	0	0.15854	1/4	0	0.16083	1/4	0	0.16497	1/4
W	(4c)	0	0.61944	1/4	0	0.61742	1/4	0	0.61468	1/4
W	(8g)	0.27161	0.89269	1/4	0.27405	0.89217	1/4	0.27863	0.89193	1/4

Structure 78: N_3W_4 in the S_3U_4 structure.[41] This is the reverse of Structure 47.

Space Group		$Pm\bar{3}m - O_h^1$ (#221)			Pearson Symbol			$cP7$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		4.23177Å	4.23177Å	4.23177Å	4.29301Å	4.29301Å	4.29301Å	4.39179Å	4.39179Å	4.39179Å
α , β , γ		90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:										
N	(3d)	1/2	0	0	1/2	0	0	1/2	0	0
W	(1a)	0	0	0	0	0	0	0	0	0
W	(3c)	0	1/2	1/2	0	1/2	1/2	0	1/2	1/2

20. N_8W_{11} structures (x = 0.57895)

Structure 79: Approximation to the δ_H^I NW structure of Khitrova and Pinsker,[37] starting with the fully occupied structure #80, doubling the unit cell in the x-y plane, and removing four of the tungsten (4f) atoms.

Space Group		$P6_3mc - C_{6v}^4$ (#186)			Pearson Symbol			$hP38$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		5.66328Å	5.66328Å	15.62088Å	5.74409Å	5.74409Å	15.85070Å	5.87612Å	5.87612Å	16.15181Å
α , β , γ		90°	90°	120°	90°	90°	120°	90°	90°	120°
Wyckoff Positions:										
N	(2b)	1/3	2/3	0.15947	1/3	2/3	0.15936	1/3	2/3	0.16031
N	(2b)	1/3	2/3	0.33553	1/3	2/3	0.33473	1/3	2/3	0.33302
N	(6c)	0.16433	0.32867	0.66521	0.16433	0.32867	0.66585	0.16367	0.32734	0.66711
N	(6c)	0.16636	0.33273	0.83940	0.16639	0.33278	0.83904	0.16650	0.33299	0.83769
W	(2b)	1/3	2/3	-0.06908	1/3	2/3	-0.06852	1/3	2/3	-0.06730
W	(2b)	1/3	2/3	0.74509	1/3	2/3	0.74520	1/3	2/3	0.74482
W	(6c)	0.16379	0.32758	0.06992	0.16365	0.32730	0.06950	0.16407	0.32814	0.06770
W	(6c)	0.16550	0.33099	0.25054	0.16534	0.33068	0.25051	0.16525	0.33050	0.25057
W	(6c)	0.16975	0.33950	0.43126	0.16989	0.33978	0.43150	0.17055	0.34110	0.43331

21. N_2W_3 structures (x = 0.600)

Structure 80: N_2W_3 constructed from the δ_H^I NW structure of Khitrova and Pinsker,[37] fully filling all sites. Structure 43 is the reverse of this structure.

Space Group		$P6_3/mmc - D_{6h}^4$ (#194)			Pearson Symbol			$hP10$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		2.85563Å	2.85563Å	15.69480Å	2.89586Å	2.89586Å	15.92167Å	2.96086Å	2.96086Å	16.24555Å
α , β , γ		90°	90°	120°	90°	90°	120°	90°	90°	120°
Wyckoff Positions:										
N	(4f)	1/3	2/3	0.66195	1/3	2/3	0.66236	1/3	2/3	0.66384
W	(2c)	1/3	2/3	1/4	1/3	2/3	1/4	1/3	2/3	1/4
W	(4f)	1/3	2/3	0.06988	1/3	2/3	0.06949	1/3	2/3	0.06807

Structure 81: N_2W_3 in the δ_R^{VI} NW structure of Khitrova and Pinsker,[37] assuming the tungsten (6c) site is fully occupied.

Space Group		$R\bar{3}m - D_{3d}^5$ (#166)			Pearson Symbol			$hR15$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		2.82823Å	2.82823Å	23.94927Å	2.86639Å	2.86639Å	24.31519Å	2.92362Å	2.92362Å	24.87295Å
α , β , γ		90°	90°	120°	90°	90°	120°	90°	90°	120°
Wyckoff Positions:										
N	(6c)	0	0	0.27238	0	0	0.27225	0	0	0.27201
W	(3a)	0	0	0	0	0	0	0	0	0
W	(6c)	0	0	0.11856	0	0	0.11868	0	0	0.11910

Structure 82: N_2W_3 structure derived from the r-W_2N_3 structure of WYL+.[33] This is the reverse of Structure 36

Space Group		$P3_1 - C_3^2$ (#144)			Pearson Symbol			$hP30$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		4.99245Å	4.99245Å	15.50163Å	5.07201Å	5.07201Å	15.67951Å	5.20586Å	5.20586Å	15.90401Å
α , β , γ		90°	90°	120°	90°	90°	120°	90°	90°	120°
Wyckoff Positions:										
N	(3a)	0.89493	0.78765	0.99630	0.89540	0.78825	0.99651	0.89564	0.78841	0.99781
N	(3a)	0.89267	0.78977	0.82174	0.89284	0.79046	0.82043	0.89311	0.79206	0.81770
N	(3a)	0.56227	0.11753	0.83379	0.56260	0.11826	0.83389	0.56235	0.11934	0.83426
N	(3a)	0.22387	0.44759	0.83437	0.22424	0.44823	0.83453	0.22452	0.44969	0.83467
W	(3a)	0.89359	0.76708	0.59175	0.89452	0.76645	0.59232	0.89629	0.76584	0.59332
W	(3a)	0.55705	0.10707	0.59061	0.55621	0.10676	0.59137	0.55336	0.10652	0.59297
W	(3a)	0.22878	0.44261	0.59051	0.23021	0.44283	0.59116	0.23398	0.44382	0.59252
W	(3a)	0.87577	0.75629	0.40835	0.87316	0.75393	0.40788	0.86571	0.74725	0.40674
W	(3a)	0.56420	0.10695	0.40838	0.56662	0.10674	0.40807	0.57432	0.10629	0.40727
W	(3a)	0.22648	0.45923	0.40821	0.22624	0.46155	0.40784	0.22561	0.46859	0.40674

Structure 83: N_2W_3 structure derived from the r-W_2N_3 structure of WYL+.[33] This is the reverse of Structure 35 We use the freedom allowed by this space group to arbitrarily set the position of one of the N (2a) atoms to the origin.

Space Group		$Cm - C_s^3$ (#8)			Pearson Symbol			$mC20$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		4.99704Å	8.66608Å	5.39929Å	5.07694Å	8.79999Å	5.46448Å	5.21065Å	9.01177Å	6.37214Å
α , β , γ		90°	107.41618°	90°	90°	107.44944°	90°	90°	56.26186°	90°
Wyckoff Positions:										
N	(2a)	0	0	0	0	0	0	0	0	0
N	(2a)	0.83602	0	0.47463	0.83553	0	0.47061	0.47385	0	0.45968
N	(4b)	0.34074	0.63509	0.51175	0.34149	0.83504	0.51200	0.33206	0.33485	0.51109
W	(2a)	0.42617	0	0.23455	0.42853	0	0.23340	0.20546	0	0.22867
W	(2a)	0.59291	0	0.78518	0.59299	0	0.78692	0.82018	0.33083	0.78451
W	(4b)	0.09974	0.83195	0.78256	0.10145	0.83165	0.78403	0.17748	0.31959	0.22759
W	(4b)	0.41072	0.32373	0.23419	0.40937	0.32269	0.23290	0.32018	0.83083	0.78451

Structure 84: N_2W_3 derived from the NaCl structure by removing 2/3 of the N atoms in the (111) plane. This is the reverse of Structure 38.

Space Group		$C2/m - C_{2h}^3$ (#12)			Pearson Symbol			$mC20$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		5.12649Å	8.86756Å	5.16084Å	5.20457Å	9.00261Å	5.23588Å	5.32803Å	9.21714Å	5.35180Å
α , β , γ		90°	109.16454°	90°	90°	109.17926°	90°	90°	109.26572°	90°
Wyckoff Positions:										
N	(2a)	0	0	0	0	0	0	0	0	0
N	(2d)	0	1/2	1/2	0	1/2	1/2	0	1/2	1/2
N	(4h)	0	0.16121	1/2	0	0.16232	1/2	0	0.16479	1/2
W	(4i)	0.28195	0	0.78064	0.28329	0	0.78136	0.28651	0	0.78245
W	(8j)	0.24927	0.17739	0.21885	0.24912	0.17786	0.21660	0.24918	0.17909	0.21199

Structure 85: N_2W_3 derived from the MoS_2 structure (#89) by removing one of the tungsten atoms. We arbitrarily set the z coordinate of the nitrogen (1a) atom to zero.

Space Group		$P3m1 - C_{3v}^1$ (#156)			Pearson Symbol			$hP5$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		2.82742Å	2.82742Å	8.43352Å	2.86730Å	2.86730Å	8.55237Å	2.92607Å	2.92607Å	8.72264Å
α , β , γ		90°	90°	120°	90°	90°	120°	90°	90°	120°
Wyckoff Positions:										
N	(1a)	0	0	0	0	0	0	0	0	0
N	(1b)	1/3	2/3	0.59188	1/3	2/3	0.59148	1/3	2/3	0.59073
W	(1a)	0	0	0.44295	0	0	0.44288	0	0	0.44195
W	(1b)	1/3	2/3	0.16594	1/3	2/3	0.16599	1/3	2/3	0.16634
W	(1b)	1/3	2/3	0.82561	1/3	2/3	0.82489	1/3	2/3	0.82249

Structure 86: N_2W_3 derived Structure 37 by reversing the positions of the nitrogen and tungsten atoms and allowing the system to relax.

Space Group		$P\bar{6}2m - D_{3h}^3$ (#189)			Pearson Symbol			$hP10$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		4.89190Å	4.89190Å	5.54435Å	4.96500Å	4.96500Å	5.61970Å	5.07225Å	5.07225Å	5.74184Å
α , β , γ		90°	90°	120°	90°	90°	120°	90°	90°	120°
Wyckoff Positions:										
W	(1a)	0	0	0	0	0	0	0	0	0
N	(1b)	0	0	1/2	0	0	1/2	0	0	1/2
N	(2d)	1/3	2/3	1/2	1/3	2/3	1/2	1/3	2/3	1/2
W	(6i)	0.66515	0	0.75843	0.66497	0	0.75914	0.66381	0	0.76090

22. N_4W_7 structures (x = 0.63636)

Structure 87: N_4W_7 structure derived from the CTi_2[35] structure by removing one of the tungsten atoms from Structure 95.

Space Group	$R3m - C_{3v}^5$ (#160)			Pearson Symbol			$hR33$		
Functional	LDA			PBE			vdW-DF2		
a , b , c	5.79011Å	5.79011Å	14.24869Å	5.87025Å	5.87025Å	14.46981Å	5.98943Å	5.98943Å	14.82145Å
α , β , γ	90°	90°	120°	90°	90°	120°	90°	90°	120°
Wyckoff Positions:									
N (3a)	0	0	0	0	0	0	0	0	0
N (9b)	0.16537	0.33074	0.83469	0.83246	0.66491	0.16809	0.83485	0.66970	0.16865
W (3a)	0	0	0.25908	0	0	0.25984	0	0	0.26117
W (9b)	0.15601	0.31202	0.58203	0.15544	0.31088	0.58162	0.15342	0.30684	0.58061
W (9b)	0.84218	0.68437	0.41765	0.84278	0.68555	0.41738	0.84490	0.68979	0.41556

23. N_8W_{15} structures (0.65217)

Structure 88: N_8W_{15} structure derived from a cI64 supercell of the NaCl structure and removing 8 N and 1 W atom. This is the same as Structure 98 with the removal of the W (2a) atom.

Space Group	$I4/mmm - D_{4h}^{17}$ (#139)			Pearson Symbol			$tI46$		
Functional	LDA			PBE			vdW-DF2		
a , b , c	8.26028Å	8.26028Å	8.14298Å	8.37655Å	8.37655Å	8.26067Å	8.55262Å	8.55262Å	8.43783Å
α , β , γ	90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:									
N (4d)	0	1/2	1/4	0	1/2	1/4	0	1/2	1/4
N (4e)	0	0	0.24086	0	0	0.24109	0	0	0.24181
N (8i)	0.24831	0	0	0.24898	0	0	0.25183	0	0
W (2b)	0	0	1/2	0	0	1/2	0	0	1/2
W (4c)	0	1/2	0	0	1/2	0	0	1/2	0
W (8h)	0.25286	0.25286	0	0.25309	0.25309	0	0.25412	0.25412	0
W (16n)	0	0.24487	0.26136	0	0.24463	0.26249	0	0.24401	0.26590

24. NW_2 structures (x = 0.66667)

Structure 89: NW_2 in the MoS_2 structure.[49] Schönfeld, Huang, and Moss refer to this as the "2H"-MoS_2 structure.[50]

Space Group	$P6_3/mmc - D_{6h}^4$ (#194)			Pearson Symbol			$hP6$		
Functional	LDA			PBE			vdW-DF2		
a , b , c	2.83728Å	2.83728Å	10.21227Å	2.87522Å	2.87522Å	10.36922Å	2.93305Å	2.93305Å	10.58384Å
α , β , γ	90°	90°	120°	90°	90°	120°	90°	90°	120°
Wyckoff Positions:									
N (2c)	1/3	2/3	1/4	1/3	2/3	1/4	1/3	2/3	1/4
W (4f)	1/3	2/3	0.61173	1/3	2/3	0.61159	1/3	2/3	0.61081

Structure 90: NW_2 in the αMoS_2 structure. Schönfeld, Huang, and Moss refer to this as the "3R"-MoS_2 structure.[50] We arbitrarily set the position of the nitrogen atom to the origin. The "α" designation is from Pearson.[36]

Space Group	$R3m - C_{3v}^5$ (#160)			Pearson Symbol			$hR9$		
Functional	LDA			PBE			vdW-DF2		
a , b , c	2.82513Å	2.82513Å	15.50656Å	2.86434Å	2.86434Å	15.72667Å	2.92087Å	2.92087Å	16.05814Å
α , β , γ	90°	90°	120°	90°	90°	120°	90°	90°	120°
Wyckoff Positions:									
N (3a)	0	0	0	0	0	0	0	0	0
W (3a)	0	0	0.24121	0	0	0.24116	0	0	0.24085
W (3a)	0	0	0.42399	0	0	0.42416	0	0	0.42481

Structure 91: NW_2 in the αSm structure.[36] This is the reverse of the structure Khitrova and Pinsker[37] call δ_R^V (#25).

Space Group	$R\bar{3}m - D_{3d}^5$ (#166)			Pearson Symbol			$hR9$		
Functional	LDA			PBE			vdW-DF2		
a , b , c	2.86587Å	2.86587Å	14.94122Å	2.90423Å	2.90423Å	15.18283Å	2.95530Å	2.95530Å	15.60398Å
α , β , γ	90°	90°	120°	90°	90°	120°	90°	90°	120°
Wyckoff Positions:									
N (3a)	0	0	0	0	0	0	0	0	0
W (6c)	0	0	0.24198	0	0	0.24172	0	0	0.24091

Structure 92: NW_2 in the Mo_2N structure.[30] This is the reverse of Structure 19.

Space Group	$I4_1/amd - D_{4h}^{19}$ (#141)			Pearson Symbol			$tI12$		
Functional	LDA			PBE			vdW-DF2		
a , b , c	4.23644Å	4.23644Å	7.89086Å	4.30206Å	4.30206Å	7.98537Å	4.41275Å	4.41275Å	8.08133Å
α , β , γ	90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:									
N (4a)	0	3/4	1/8	0	3/4	1/8	0	3/4	1/8
M (8e)	0	3/4	0.89014	0	3/4	0.89096	0	3/4	0.89469

Structure 93: NW_2 constructed by removing 16 N atoms from a 64 atom supercell of the NaCl structure. This is the reverse of Structure 27.

Space Group	$Pm\bar{3}m - O_h^1$ (#221)			Pearson Symbol			$cI36$		
Functional	LDA			PBE			vdW-DF2		
a , b , c	8.30045Å	8.30045Å	8.30045Å	8.42147Å	8.42147Å	8.42147Å	8.60415Å	8.60415Å	8.60415Å
α , β , γ	90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:									
N (1a)	0	0	0	0	0	0	0	0	0
N (3c)	0	1/2	1/2	0	1/2	1/2	0	1/2	1/2
N (12i)	0	0.24789	0.24789	0	0.24749	0.24749	0	0.24703	0.24703
W (6e)	0	0	0.27632	0	0	0.27708	0	0	0.27753
W (6f)	0.24987	1/2	1/2	0.24956	1/2	1/2	0.24949	1/2	1/2
W (8g)	0.26719	0.26719	0.26719	0.26812	0.26812	0.26812	0.27078	0.27078	0.27078
W (12h)	0.23775	0	1/2	0.23709	0	1/2	0.23488	0	1/2

Structure 94: NW_2 constructed by removing 4 N atoms from a cF64 supercell of the NaCl structure.

Space Group	$Imma - D_{2h}^{28}$ (#74)			Pearson Symbol			$oI24$		
Functional	LDA			PBE			vdW-DF2		
a , b , c	5.78488Å	8.33312Å	5.94700Å	5.85966Å	8.46492Å	6.03547Å	5.96447Å	8.68101Å	6.17371Å
α , β , γ	90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:									
N (4a)	0	0	0	0	0	0	0	0	0
N (4c)	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4
N (4e)	0	1/4	-0.03099	0	1/4	-0.03220	0	1/4	-0.03355
W (4e)	0	1/4	0.50858	0	1/4	0.50860	0	1/4	0.50108
W (8g)	1/4	-0.01560	1/4	1/4	-0.01676	1/4	1/4	-0.02014	1/4

Structure 95: NW_2 in the CTi_2 structure.[35] Suetin, Shein, and Ivanovskii[51] used this to approximate Hägg's β-NW_2 structure.[52]

Space Group	$Fd\bar{3}m - O_h^7$ (#227)			Pearson Symbol			$hR33$		
Functional	LDA			PBE			vdW-DF2		
a , b , c	8.28537Å	8.28537Å	8.28537Å	8.40523Å	8.40523Å	8.40523Å	8.58784Å	8.58784Å	8.58784Å
α , β , γ	90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:									
N (16c)	0	0	0	0	0	0	0	0	0
W (32e)	0.25837	0.25837	0.25837	0.25880	0.25880	0.25880	0.26006	0.26006	0.26006

Structure 96: NW_2 in the PbO_2 structure,[32] with W on the O sites. This is the reverse of structure #21.

Space Group	$Pbcn - D_{2h}^{14}$ (#60)			Pearson Symbol			$oP12$		
Functional	LDA			PBE			vdW-DF2		
a , b , c	4.83239Å	5.95042Å	5.00862Å	4.89864Å	6.04021Å	5.08151Å	5.02832Å	6.17785Å	5.16528Å
α , β , γ	90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:									
N (4c)	0	0.38449	1/4	0	0.36342	1/4	0	0.39007	1/4
W (8d)	0.25662	0.36459	0.59586	0.25683	0.36342	0.59726	0.25909	0.36101	0.60113

Structure 97: NW_2 constructed by removing 16 W atoms from a 64 atom supercell of the NaCl structure. This is the reverse of Structure 28.

Space Group	$Pm\bar{3}m - O_h^1$ (#221)			Pearson Symbol			$cI36$		
Functional	LDA			PBE			vdW-DF2		
a , b , c	8.30145Å	8.30145Å	8.30145Å	8.42169Å	8.42169Å	8.42169Å	8.60530Å	8.60530Å	8.60530Å
α , β , γ	90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:									
N (1a)	0	0	0	0	0	0	0	0	0
N (3c)	0	1/2	1/2	0	1/2	1/2	0	1/2	1/2
N (12j)	1/2	0.25004	0.25004	1/2	0.25037	0.25037	1/2	0.25139	0.25139
W (6e)	0	0	0.24974	0	0	0.24959	0	0	0.24993
W (6f)	0.26765	1/2	1/2	0.26841	1/2	1/2	0.27005	1/2	1/2
W (8g)	0.23621	0.23621	0.23621	0.23542	0.23542	0.23542	0.23283	0.23283	0.23283
W (12h)	0.23520	0	1/2	0.23460	0	1/2	0.23275	0	1/2

Structure 98: NW_2 structure derived from a cI64 supercell of the NaCl structure and removing 8 N atoms. Eliminating the W (2a) atom leads to Structure 88.

Space Group		$I4/mmm - D_{4h}^{17}$ (#139)			Pearson Symbol			$tI46$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		8.30627Å	8.30627Å	8.30396Å	8.41843Å	8.41843Å	8.44457Å	8.57784Å	8.57784Å	8.70889Å
α , β , γ		90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:										
N	(4d)	0	1/2	1/4	0	1/2	1/4	0	1/2	1/4
N	(4e)	0	0	0.25218	0	0	0.25186	0	0	0.25086
N	(8i)	0.25079	0	0	0.25050	0	0	0.24953	0	0
W	(2a)	0	0	0	0	0	0	0	0	0
W	(2b)	0	0	1/2	0	0	1/2	0	0	1/2
W	(4c)	0	1/2	0	0	1/2	0	0	1/2	0
W	(8h)	0.26075	0.26705	0	0.26136	0.26136	0	0.26320	0.26320	0
W	(16n)	0	0.25014	0.26680	0	0.25017	0.26848	0	0.25002	0.27413

Structure 99: NW_2 structure derived from a cF64 supercell of the NaCl structure by removing 4 N atoms.

Space Group		$P4/mmm - D_{4h}^{1}$ (#123)			Pearson Symbol			$tP3$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		2.95024Å	2.95024Å	4.13872Å	2.99277Å	2.99277Å	4.19568Å	3.05793Å	3.05793Å	4.28527Å
α , β , γ		90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:										
N	(1a)	0	0	0	0	0	0	0	0	0
W	(1b)	0	0	1/2	0	0	1/2	0	0	1/2
W	(1c)	1/2	0	0	1/2	0	0	1/2	0	0

Structure 100: NW_2 constructed by removing 14 atoms from a cI64 supercell of the NaCl structure. This is the reverse of Structure 15.

Space Group		$Im\bar{3}m - O_h^9$ (#229)			Pearson Symbol			$cI36$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		7.94613Å	7.94613Å	7.94613Å	8.06722Å	8.06722Å	8.06722Å	8.22260Å	8.22260Å	8.22260Å
α , β , γ		90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:										
N	(12d)	1/2	1/4	0	1/2	1/4	0	1/2	1/4	0
W	(24h)	0	0.25391	0.25391	0	0.25332	0.25332	0	0.25432	0.25432

Structure 101: NW_2 in the δ_H^{II} structure of Khitrova and Pinsker.[37] Although they list the space group as $P\overline{3}$ rather than $P\overline{3}m1$, for these Wyckoff positions the space groups are identical. We choose the higher symmetry of the $P\overline{3}m1$ space group.

Space Group		$P\overline{3}m1 - D_{3d}^3$ (#164)			Pearson Symbol			$hP9$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		2.79023Å	2.79023Å	17.42820Å	2.83718Å	2.83718Å	17.65225Å	2.90362Å	2.90362Å	17.98092Å
α , β , γ		90°	90°	120°	90°	90°	120°	90°	90°	120°
Wyckoff Positions:										
N	(1b)	0	0	1/2	0	0	1/2	0	0	1/2
N	(2d)	1/3	2/3	0.15081	1/3	2/3	0.15041	1/3	2/3	0.15010
W	(2c)	0	0	0.07588	0	0	0.07574	0	0	0.07533
W	(2d)	1/3	2/3	0.26246	1/3	2/3	0.26211	1/3	2/3	0.26146
W	(2d)	1/3	2/3	0.41752	1/3	2/3	0.41731	1/3	2/3	0.41630

25. N_2W_5 structures (x = 0.71429)

Structure 102: N_2W_5 derived from the MoS_2 structure (#89) by adding a tungsten atom between the WNW layers.

Space Group		$P(-3)m1 - D_{3d}^3$ (#164)			Pearson Symbol			$hP7$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		2.82241Å	2.82241Å	12.68652Å	2.86114Å	2.86114Å	12.87430Å	2.91671Å	2.91671Å	13.13813Å
α , β , γ		90°	90°	120°	90°	90°	120°	90°	90°	120°
Wyckoff Positions:										
N	(2d)	1/3	2/3	0.70153	1/3	2/3	0.70153	1/3	2/3	0.70184
W	(1a)	0	0	0	0	0	0	0	0	0
W	(2d)	1/3	2/3	0.18613	1/3	2/3	0.18624	1/3	2/3	0.18578
W	(2d)	1/3	2/3	0.59003	1/3	2/3	0.58975	1/3	2/3	0.58893

26. NW_3 structures (x = 0.750)

Structure 103: NW_3 starting in the Molybdite (MoO_3) structure.[20] This is reverse of Structure 9. However, upon relaxation, the structure relaxed to the slightly higher symmetry Cmcm structure for all functionals.

Space Group		$Cmcm - D_{2h}^{17}$ (#63)			Pearson Symbol			$oC16$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		4.17491Å	11.85749Å	4.15521Å	4.23377Å	12.03819Å	4.21354Å	4.32374Å	12.30623Å	4.29525Å
α , β , γ		90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:										
N	(4c)	0	0.07793	1/4	0	0.07740	1/4	0	0.07631	1/4
W	(4c)	0	0.89899	1/4	0	0.89812	1/4	0	0.89586	1/4
W	(4c)	0	0.25537	1/4	0	0.25519	1/4	0	0.25597	1/4
W	(4c)	0	0.58553	1/4	0	0.58546	1/4	0	0.24403	1/4

Structure 104: NW_3 in the P_3Tc structure.[21] This is the reverse Structure 10.

Space Group		$Pnma - D_{2h}^{16}$ (#62)			Pearson Symbol			$oP16$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		15.70481Å	2.91338Å	4.58860Å	15.96981Å	2.93765Å	4.66695Å	16.53087Å	2.89162Å	4.87654Å
α , β , γ		90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:										
N	(4c)	0.33577	1/4	0.01072	0.16409	1/4	0.48794	0.33615	1/4	0.02501
N	(4c)	0.11509	1/4	0.23295	0.05190	1/4	0.23991	0.44759	1/4	0.26097
W	(4c)	0.44832	1/4	0.25991	0.38582	1/4	0.26846	0.10981	1/4	0.23092
W	(4c)	0.22327	1/4	0.76812	0.27546	1/4	0.73136	0.22913	1/4	0.78258

27. NW_4 structures (x = 0.800)

Structure 105: NW_4 in the ReP_4 structure.[17] This is the reverse of Structure 7.

Space Group		$Pbca - D_{2h}^{15}$ (#61)			Pearson Symbol			$oP40$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		11.56201Å	5.00816Å	9.29737Å	11.73041Å	5.08234Å	0.94300	12.69788Å	5.78622Å	9.06069Å
α , β , γ		90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:										
N	(8c)	0.06171	0.42239	0.37980	0.06152	0.57726	0.62045	0.18599	0.05368	0.82812
W	(8c)	0.19046	0.60451	0.25656	0.19035	0.10609	0.24324	0.19797	0.42207	0.44870
W	(8c)	0.18778	0.24660	0.50515	0.18735	0.75307	0.49516	0.09739	0.93228	0.49969
W	(8c)	0.06899	0.77376	0.50302	0.06922	0.22590	0.49663	0.03434	0.38998	0.69789
W	(8c)	0.06849	0.08909	0.24816	0.06898	0.58966	0.25204	0.00930	0.07678	0.64496

28. W structures (x = 1)

Structure 106: Body-centered cubic tungsten, the ground state structure.

Space Group		$Im\bar{3}m - O_h^9$ (#229)			Pearson Symbol			$cI2$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		3.14264Å	3.14264Å	3.14264Å	3.18934Å	3.18934Å	3.18934Å	3.25029Å	3.25029Å	3.25029Å
α , β , γ		90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:										
W	(2a)	0	0	0	0	0	0	0	0	0

Structure 107: The β-W (A15) structure.

Space Group		$Pm\bar{3}n - O_h^3$ (#223)			Pearson Symbol			$cP8$		
Functional		LDA			PBE			vdW-DF2		
a , b , c		5.01509Å	5.01509Å	5.01509Å	5.08919Å	5.08919Å	5.08919Å	5.18500Å	5.18500Å	5.18500Å
α , β , γ		90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:										
W	(2a)	0	0	0	0	0	0	0	0	0
W	(6d)	0	1/4	1/2	0	1/4	1/2	0	1/4	1/2

Structure 108: Face-centered cubic tungsten.

Space Group	$Fm\bar{3}m - O_h^5$ (#225)			Pearson Symbol			$cF4$		
Functional	LDA			PBE			vdW-DF2		
a , b , c	3.98139Å	3.98139Å	3.98139Å	4.04310Å	4.04310Å	4.04310Å	4.12107Å	4.12107Å	4.12107Å
α , β , γ	90°	90°	90°	90°	90°	90°	90°	90°	90°
Wyckoff Positions:									
W (4a)	0	0	0	0	0	0	0	0	0

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